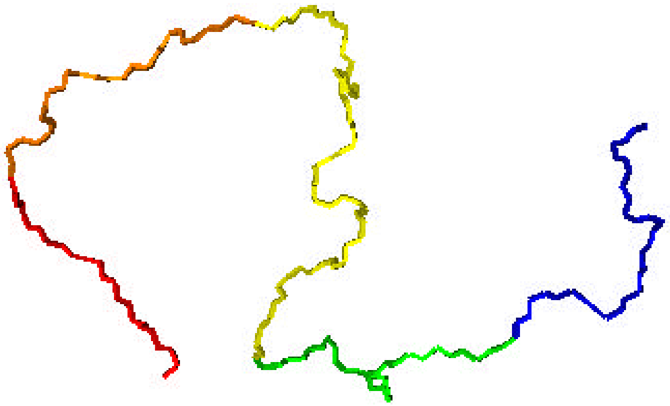
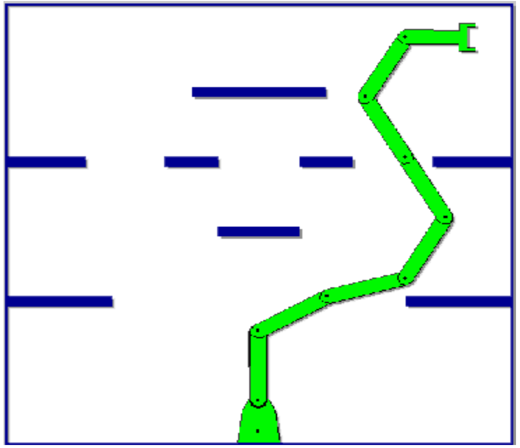
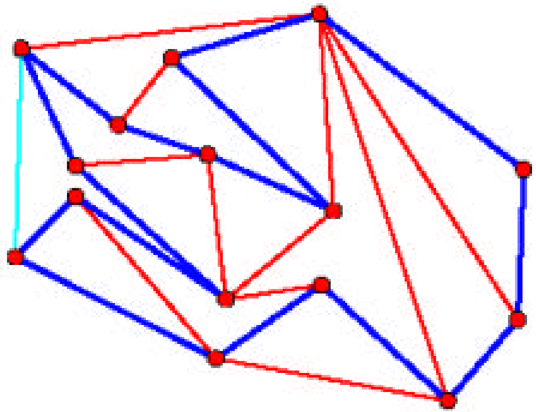






Folding and Unfolding of Polygonal Linkages

Ileana Streinu

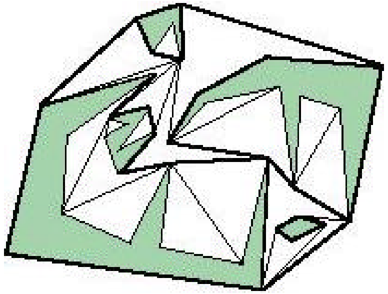
Computer Science Department

Smith College, MA

streinu@cs.smith.edu

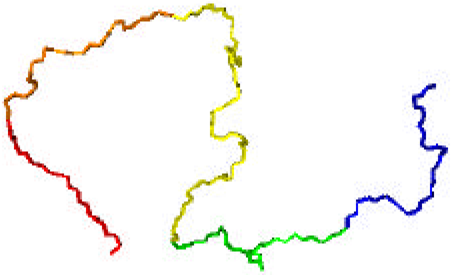
http://cs.smith.edu/~streinu

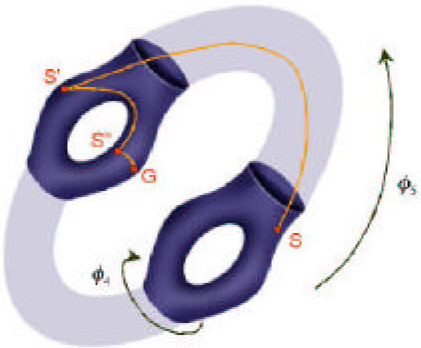
CARGO Project Members



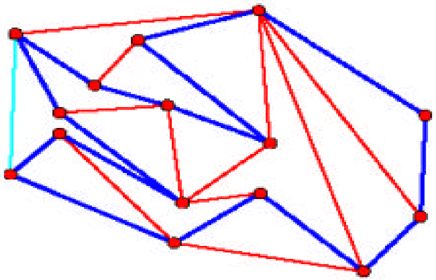
Leonidas Guibas, CS Stanford

Michael Levitt, Structural Biology Stanford





R. James Milgram, Math Stanford

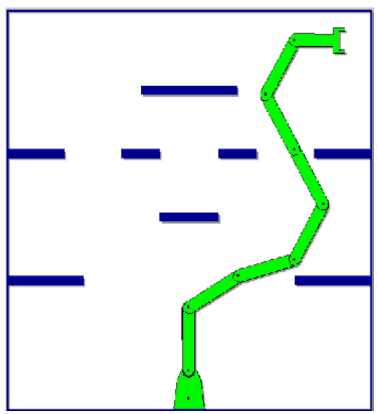


Ileana Streinu, CS Smith

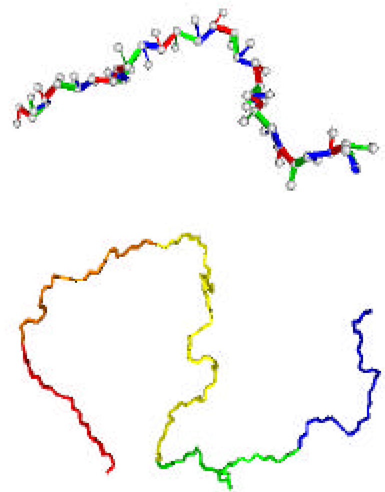
Motivation

Mathematical Foundations of Folding and Unfolding Processes for:

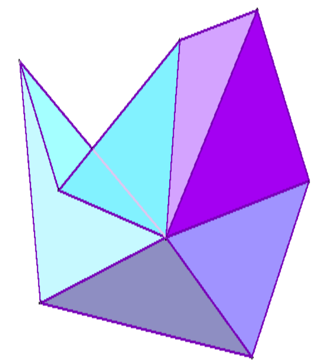
Carpenter's Rules



Robot arms



Proteins



Origamis

Our Long term goal:

understanding the mathematical and algorithmic foundations of the

Protein Folding problem

"One of the premier problems in science …"

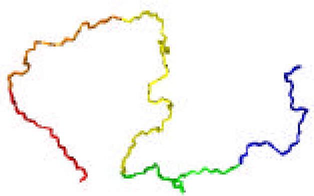
R. Karp, Mathematical Challenges from Genomics and Molecular Biology, Notices AMS, May 2002

From Vijay Pande's Folding@Home page at Stanford

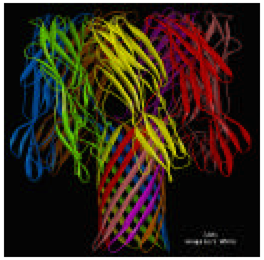
Our Long term goal:

(beyond the range of this CARGO Incubation Grant)

understanding the mathematical and algorithmic foundations of the



Protein Folding problem



•The **geometry of protein molecules** can be accurately modeled as a linear

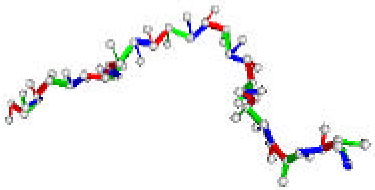
3-d polygonal linkage with fixed edge lengths

(the bond lengths) and vertex angles (the bond angles).

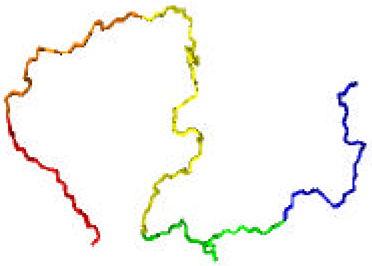
•Used with general *self-avoidance* and *repulsive and attractive interactions* between the vertices, the model is good enough to study **protein folding processes, protein fold prediction, loop conformations** (e.g. in antibodies) and conformational changes (general changes in structure).

•So far studied by a **wide array of simulations** and heuristics

•Very recently the problem has been seen to have deep connections to computer science (particularly **computational geometry**) and mathematics (particularly **topology**).



Outline



- Quick overview of current approaches
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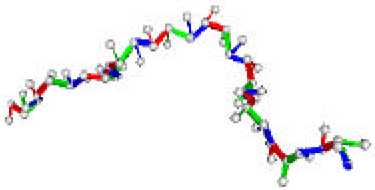
- What we plan to do
- Overview of the pseudo-triangulation approach to the 2 dimensional problem
- Lessons learned from 2d
- Challenges in dimension 3



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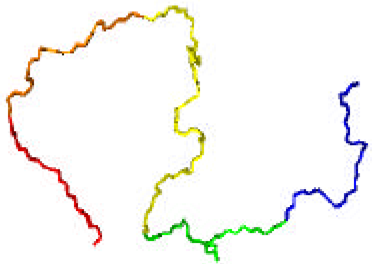

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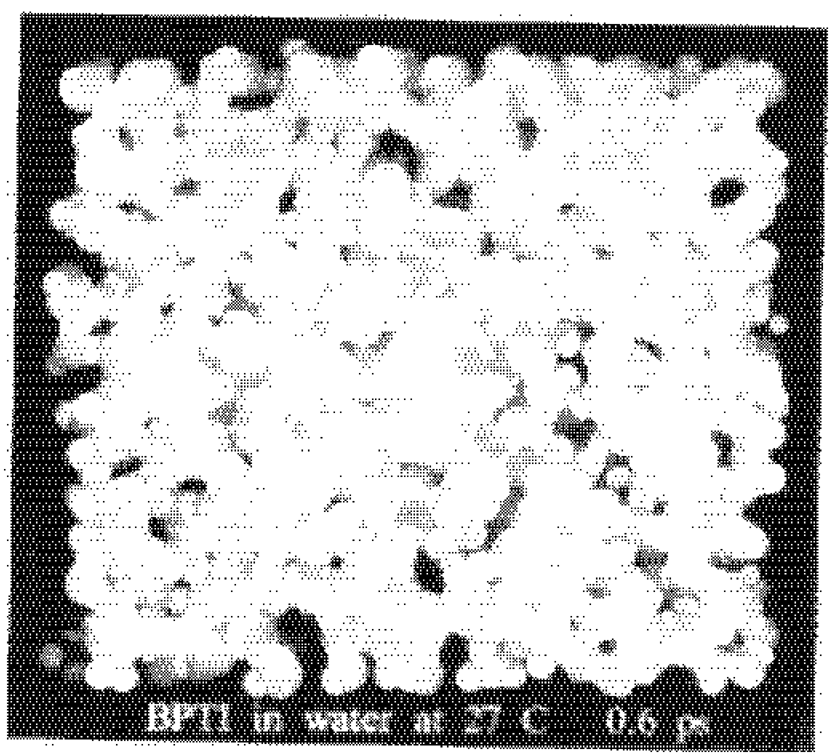
Simulating Protein Folding

From M. Levitt's MSRI lecture, 2000

SIMULATING FOLDING

PHYSICS



- 10,000 particles
- Partial Differential Equations
- $10^9 - 10^{12}$ Time Steps ($10^3 - 10^6$ days)

•Partial Differential Equations

•For 10,000 particles

•$10^9 – 10^{12}$ time steps ($10^3 – 10^6$ days)

Simulating Protein Folding

- "Ensemble Dynamics"
- Distributed computations over thousands of computers worldwide
- Simulates several potential trajectories, tried independently

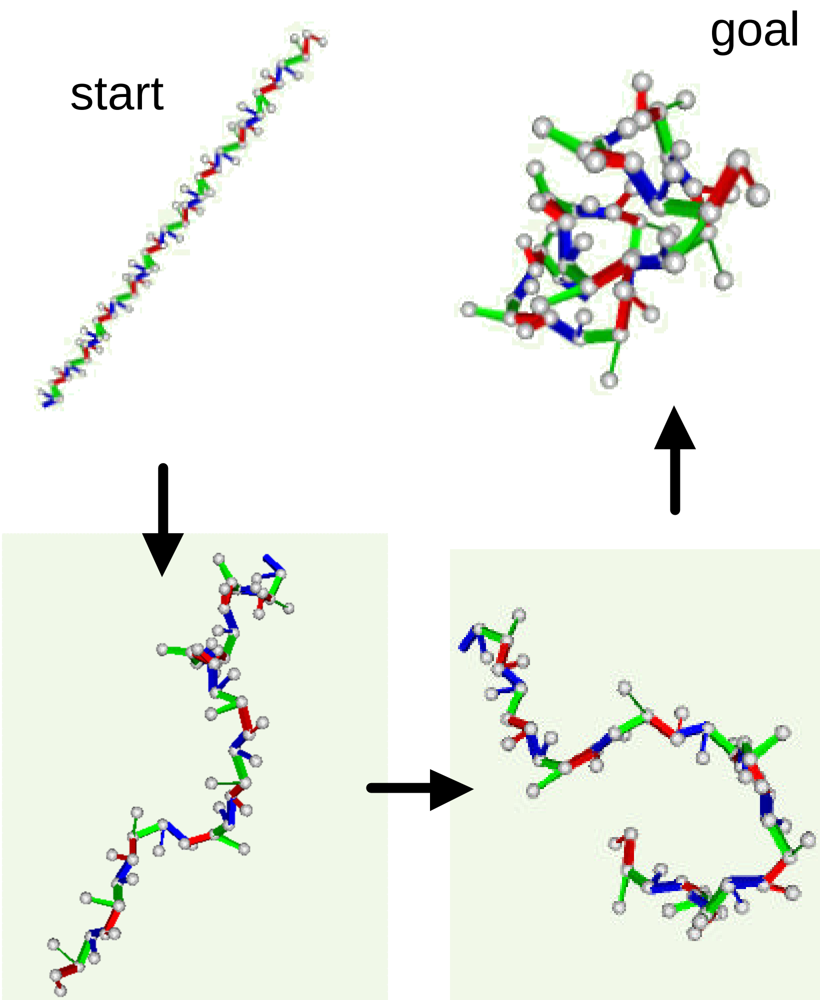
A simple ALPHA-helix, from Vijay Pande's Folding@Home page at Stanford

Computational Geometry

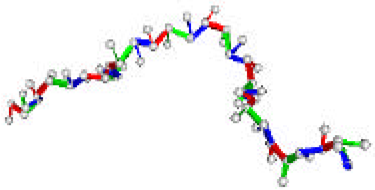
Previous Work on Folding Processes (when Start and Goal conformations are known) using modified

Probabilistic Roadmaps

(from Nancy Amato's group at Texas A&M)



- PRM approach (Kavraki Latombe Overmars Svestka '96)
- Generate random points in configuration space
- Add start and goal to roadmap
- Extract energetically most feasible between them



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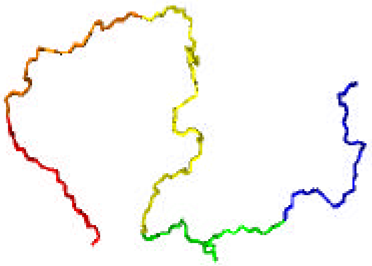

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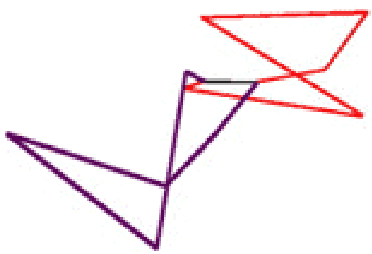
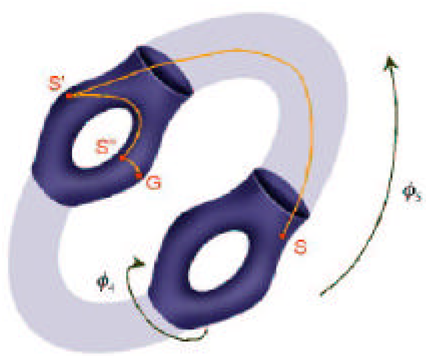
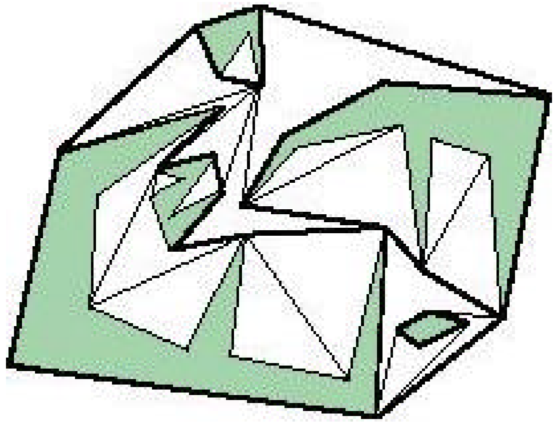
Topology of Configuration Space of Linkages



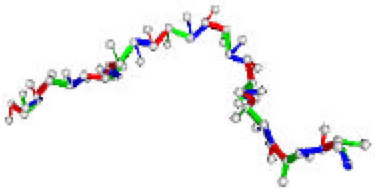
- 2d Milgram and Trinkle'01, 3d Milgram'02
- Allow crossings in reconfiguration of linkage
- Complete description of topological structure: boundaries of unions of $(S^1)^k \times I^{n-1-k}$
- Study singularities. Global trajectory guided by singularity avoidance. [Other approach, based on line-tracking motions: Lenhart and Whitesides]
- Show avi file

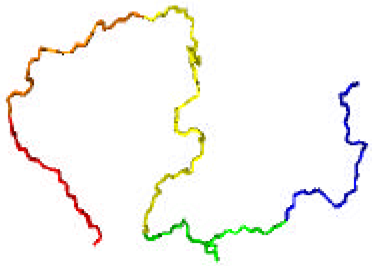


Kinetic Data Structures are Designed for Efficient Processing of Points in Motion



- Guibas' group at Stanford (et al.)
- Maintain a sparse tiling of the free space between obstacles and the moving objects
- Use pseudo-triangulations
- Very efficient





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Our Proposed Mathematical and Algorithmic Approach

(beyond the range of this one year CARGO Incubation Grant)

Study the topology and algorithmics of

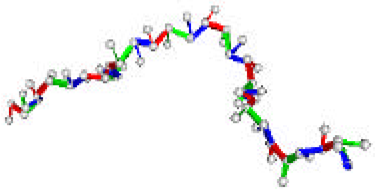
folding processes of **2d and 3d linkages**

Goal: Develop a discrete (combinatorially described) partitioning of configuration space which may be more easily sampled to generate candidates for folded states [compare with PRM]

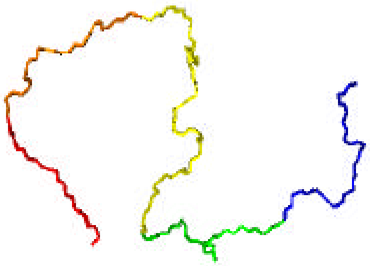
- Use recently developed ideas from 2d based on Pseudo-triangulations and Rigidity Theoretical tools
- Tools: "3d pseudo-triangulations"?
- Simplify the numerical computations using tools from combinatorial Rigidity Theory
- Explore potential parallelism

What we plan to do within the one-year of the CARGO incubation grant

- IS spends a Fall'02 sabbatical at Stanford
- Collaborate with the other PIs on:
  - Fundamental Question: combinatorics of 3d expansive motions.
  - Data Structures: what are 3d pseudo-triangulations?
  - Topology: partition configuration space into regions with predictable expansion properties (2 and 3d). Impact of singularities. Impact of fixed crossings on predictable expansive/contractive motions.
  - Study feasibility of extending current 2d implementations in contractive (rather than expansive) fashion, and to 3d
  - Study feasibility of applying to biology
- Collaboration may extend beyond this preliminary phase only through involvement of PhD students



Outline of the Talk



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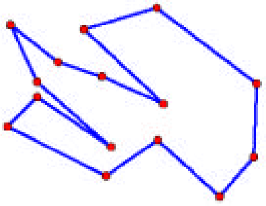
Previous and current work (IS'00,'01,'02) on the pseudo-triangulation approach:

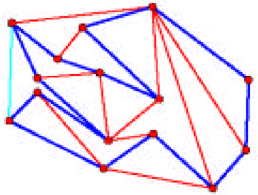
- A surprisingly simple and efficient algorithmic approach for the planar case.
- Based on motions that are expansive: they guarantee self-avoidance by increasing all distances between pairs of points. Can be computed locally.
- Simple mechanisms with only one degree of freedom guide the arm in its global unfolding.
- Resulting unfolding process: at most $O(n^3)$ steps (provable; in practice $O(n)$ observed) each computable in at most $O(n)$ time.
- Space of pseudo-triangulation: exponential in size, but seems amenable to simple sampling due to clean combinatorial structure
- Ideas for simplifying the numerical computations
- Ideas for parallelizing certain parts of the computation

Main Idea:



Linkages have too many degrees of freedom.

Planning their motions requires very complex strategies for simultaneously controlling all joints and avoiding collisions.



Pseudo-triangulation approach:

- Add extra bars to reduce the degrees of freedom
- Pseudo-triangulations with a CH edge removed are simple expansive mechanisms with only one degree of freedom that can be used to guide the global folding and unfolding of the linkage.

The Carpenter's Rule Problem

Can every simple planar polygonal linkage be convexified (in the plane) without collisions?

History:

1970's Topology community: Bergman, Schanuel, Grenader (cf. R. Kirby, Problems in Low dimensional Topology, 1995)

Early 1990's Computer Science community: W. Lenhart and Sue Whitesides, J. Mitchell.

Barbados workshop 1998: T. Biedl, E. Demaine, M. Demaine, S. Lazard, A. Lubiw, J. O'Rourke, M. Overmars, S. Robbins, I.S., G. Toussaint, S. Whitesides. Various special cases.

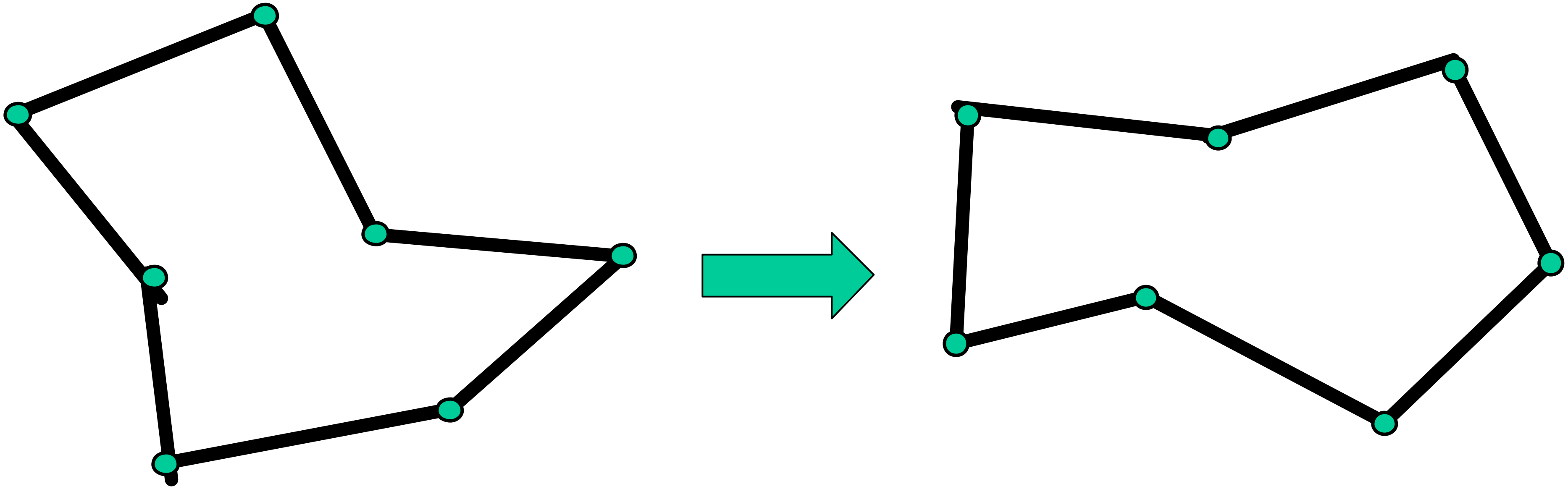
Others '99 J. Erickson, B. Aronov, J.E. Goodman, R. Pollack etc.

G. Rote, NSF Monte Verita workshop 1999, LP and expansive motions.

R.Connelly, E.Demaine, G. Rote 2000: YES! Answer: Always.

I.Streinu 2000: A more algorithmic solution based on pseudo-triangulations.

Planar linkage reconfiguration



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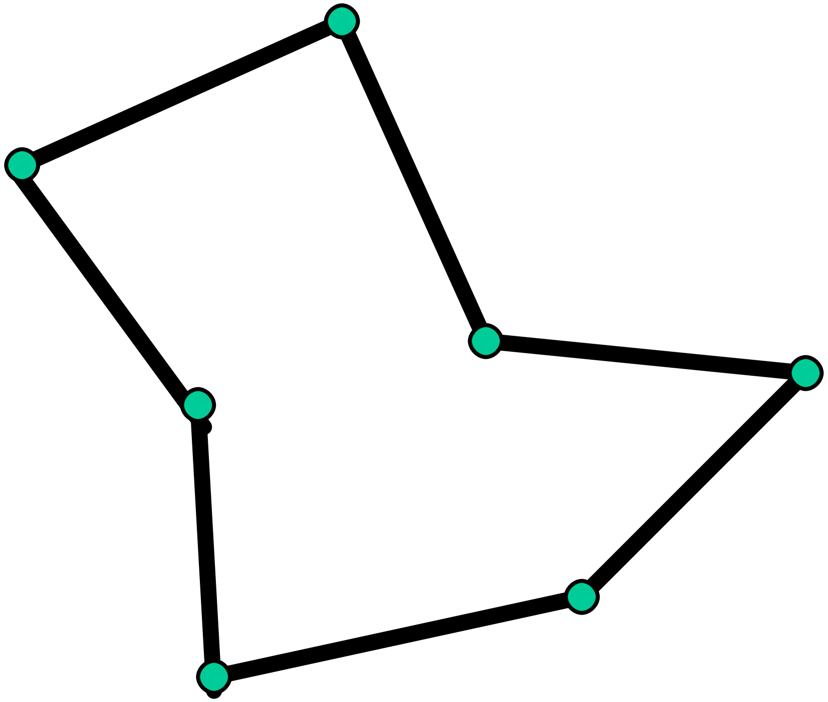
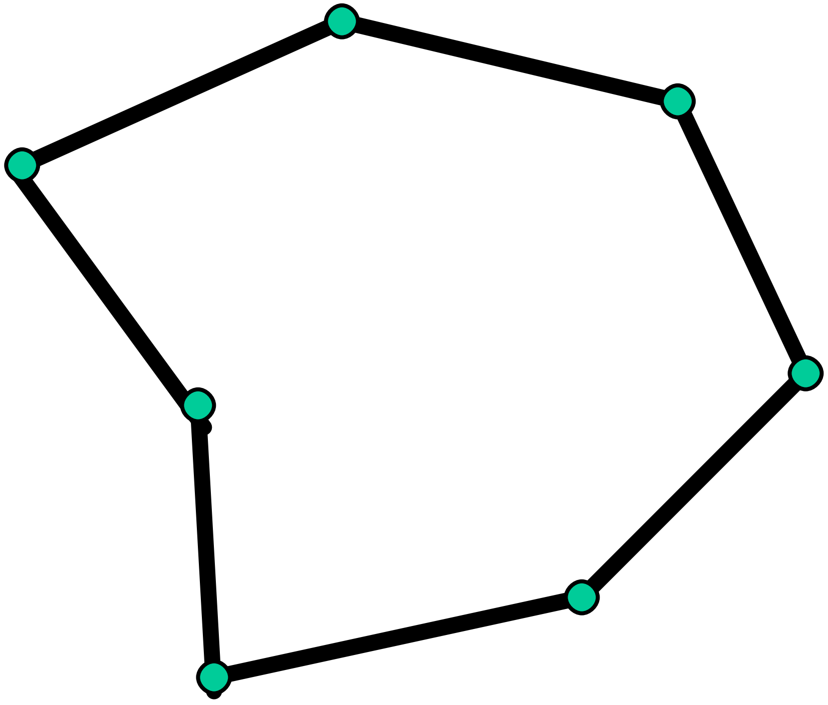


Planar linkage reconfiguration



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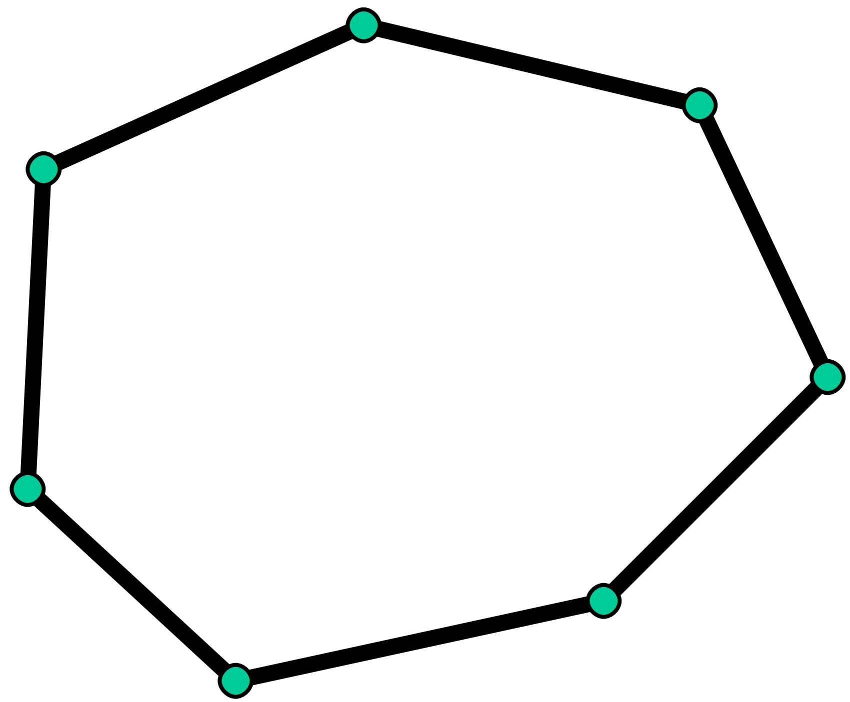
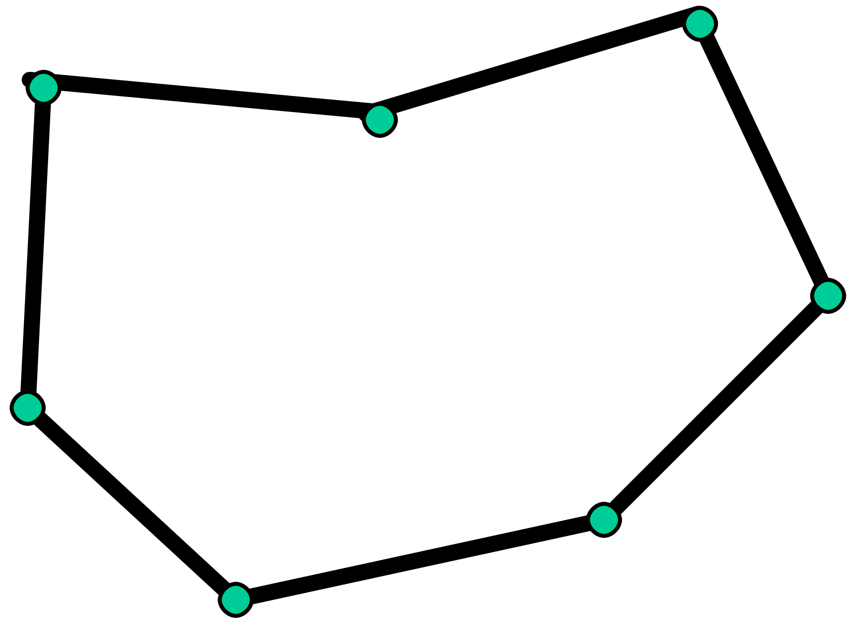


Intermediate state:
Convex Polygon

Planar linkage reconfiguration



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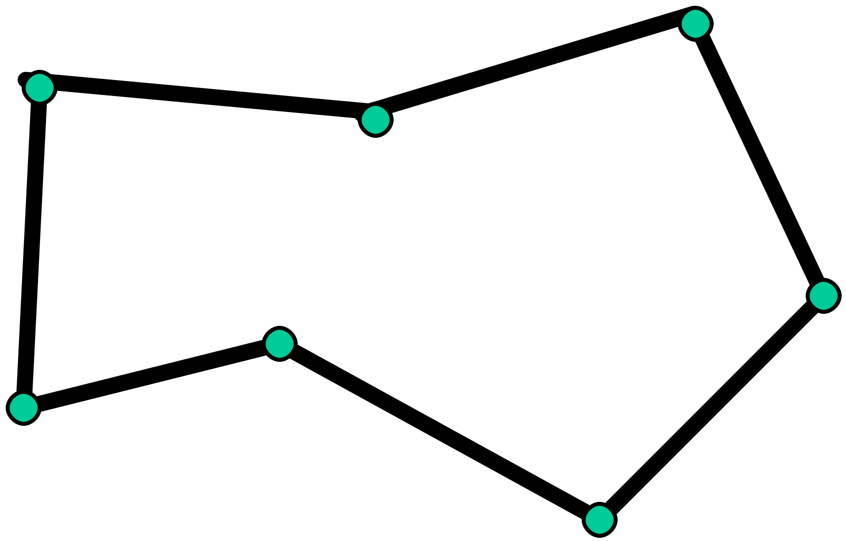
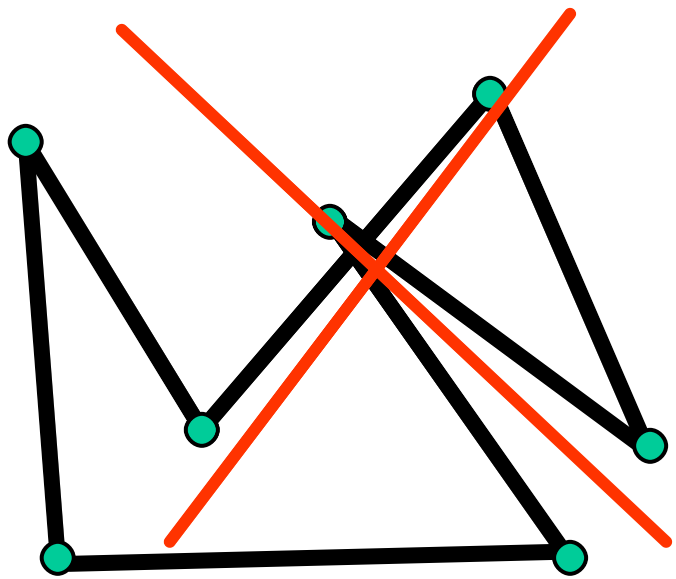
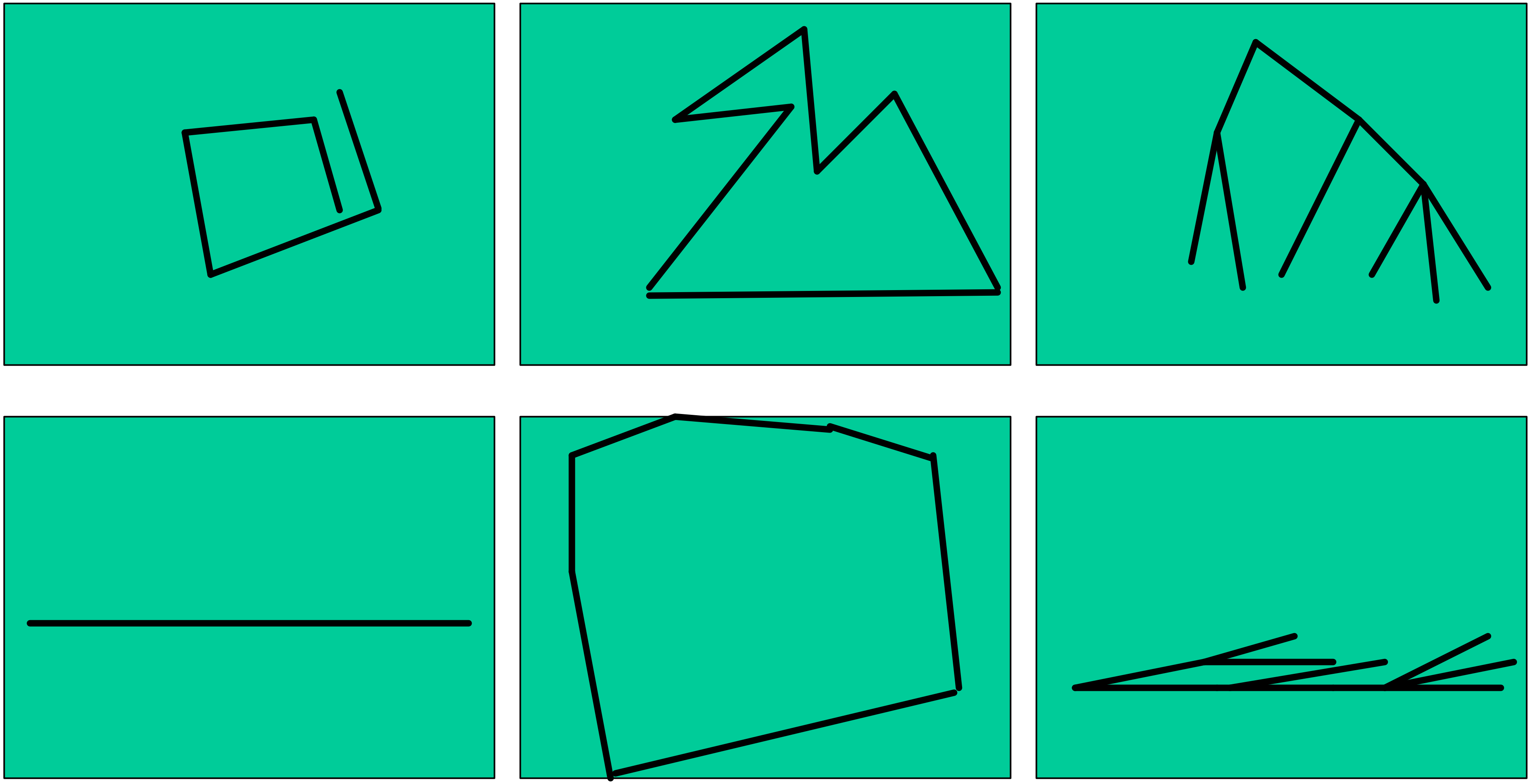


Permissible Motions

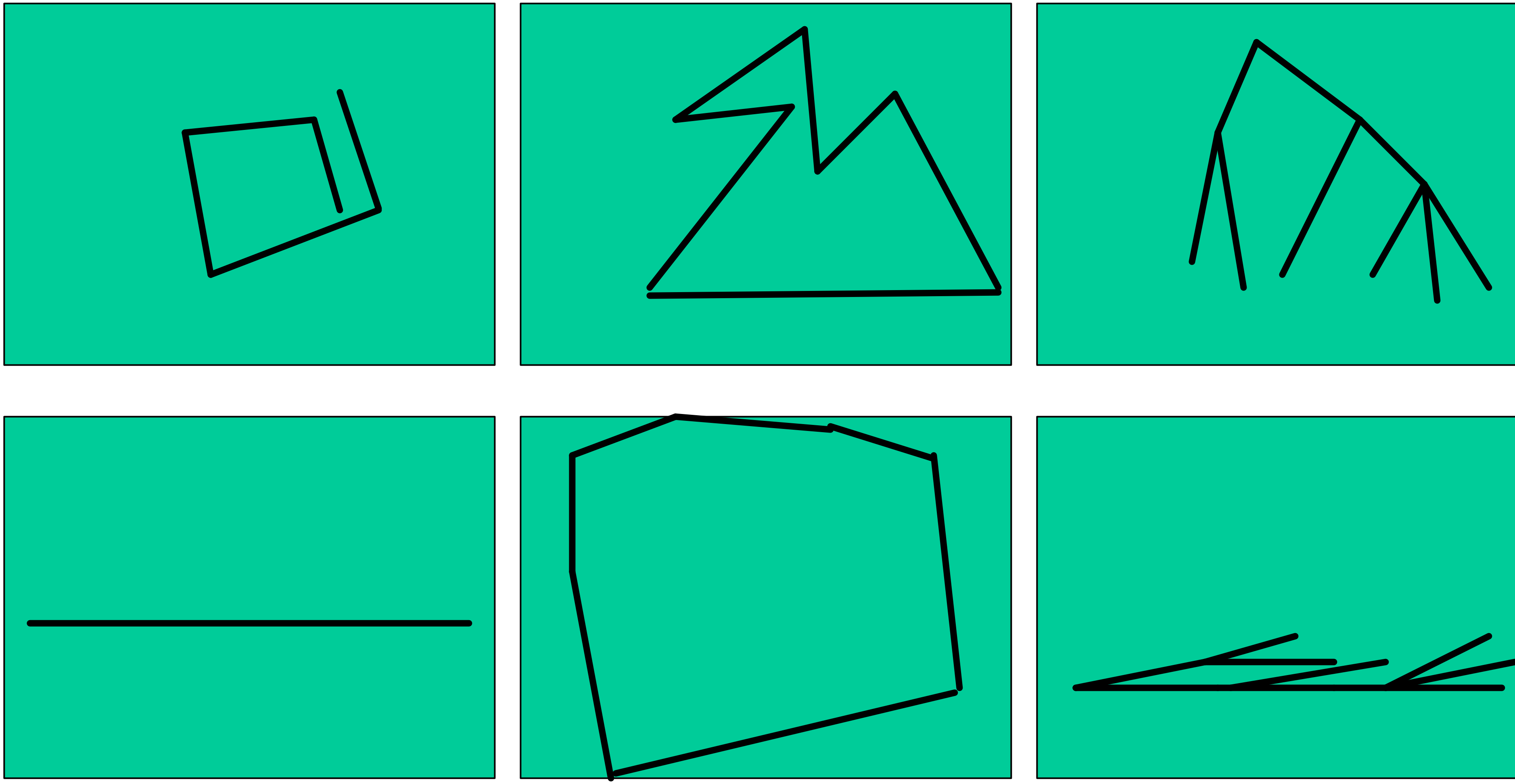


No intersections of bars are allowed during the motion

Move continuously to a canonical form

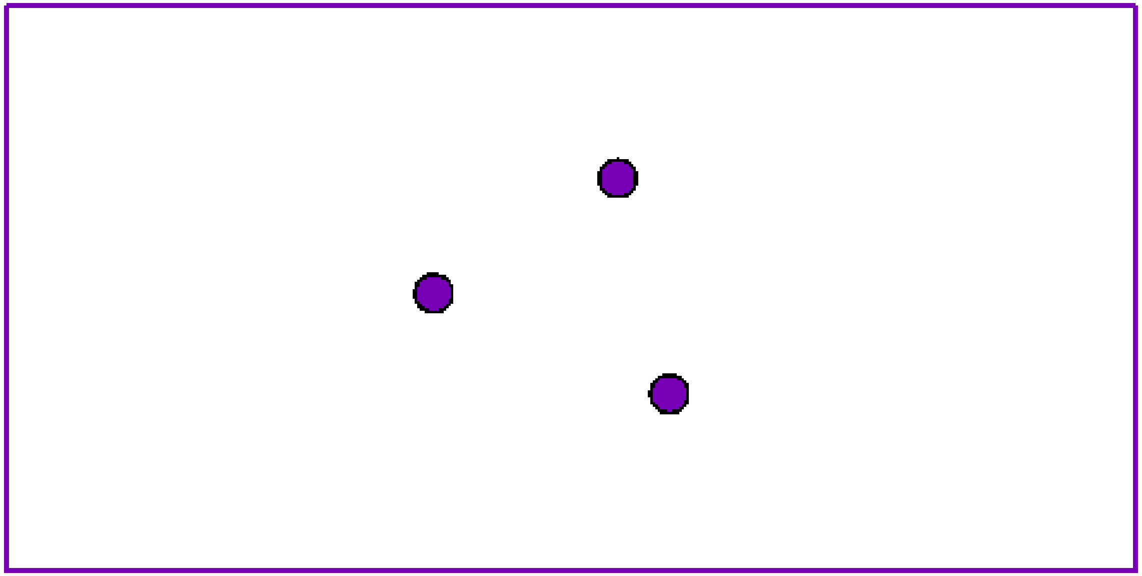


Collision-free Configuration Space: connected?



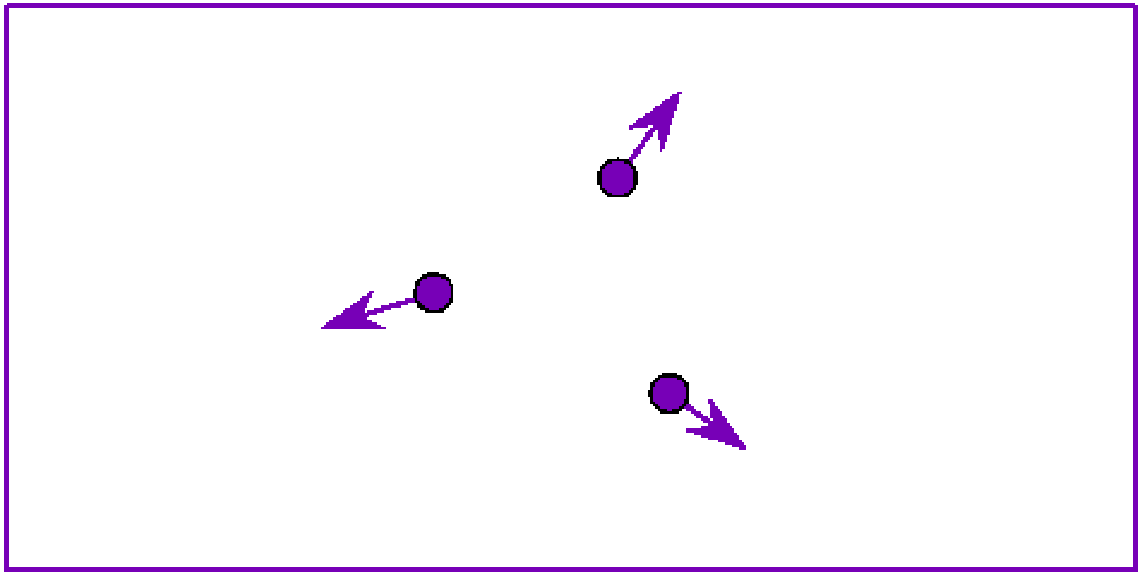
Yes Yes No

Avoiding Collisions via Expansive Motions



All pairwise distances increase (or stay the same)

Avoiding Collisions via Expansive Motions



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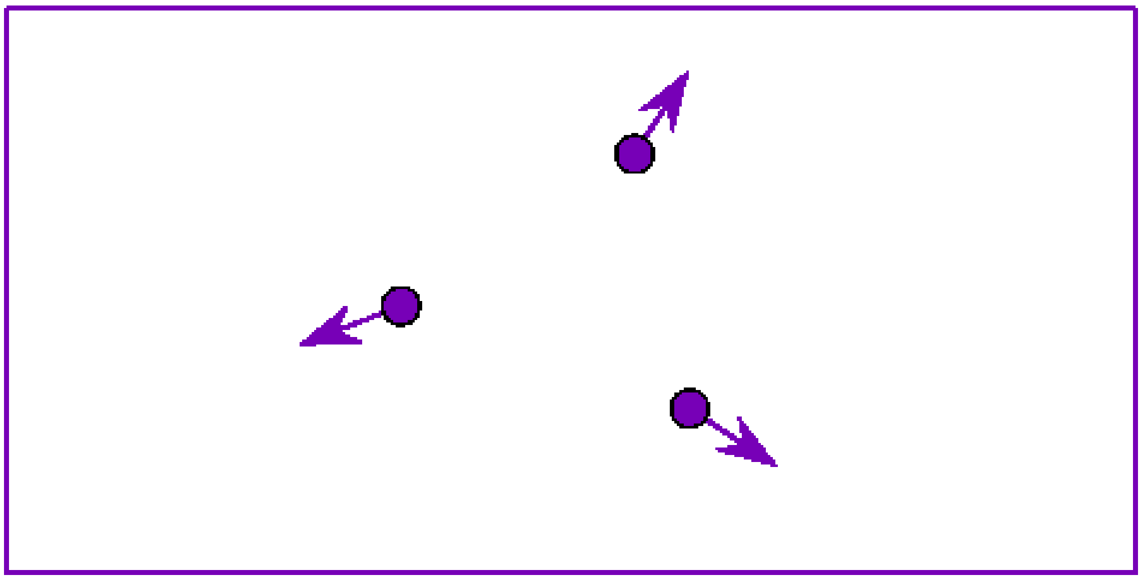

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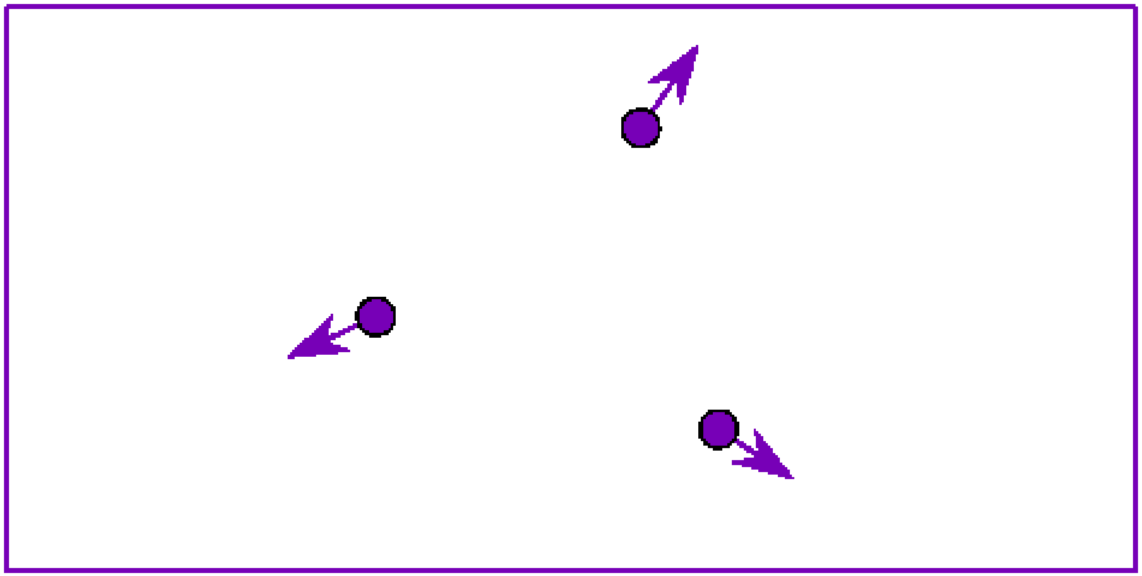
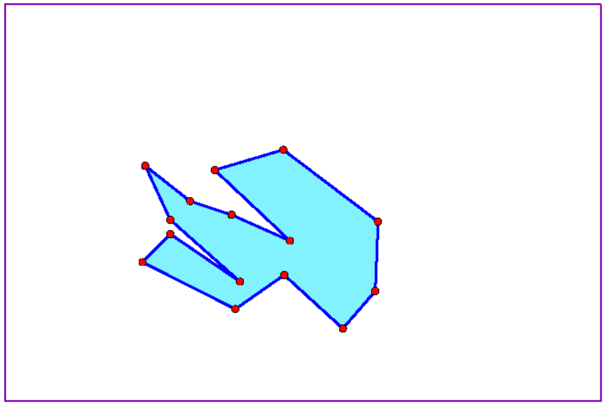


All pairwise distances increase (or stay the same)

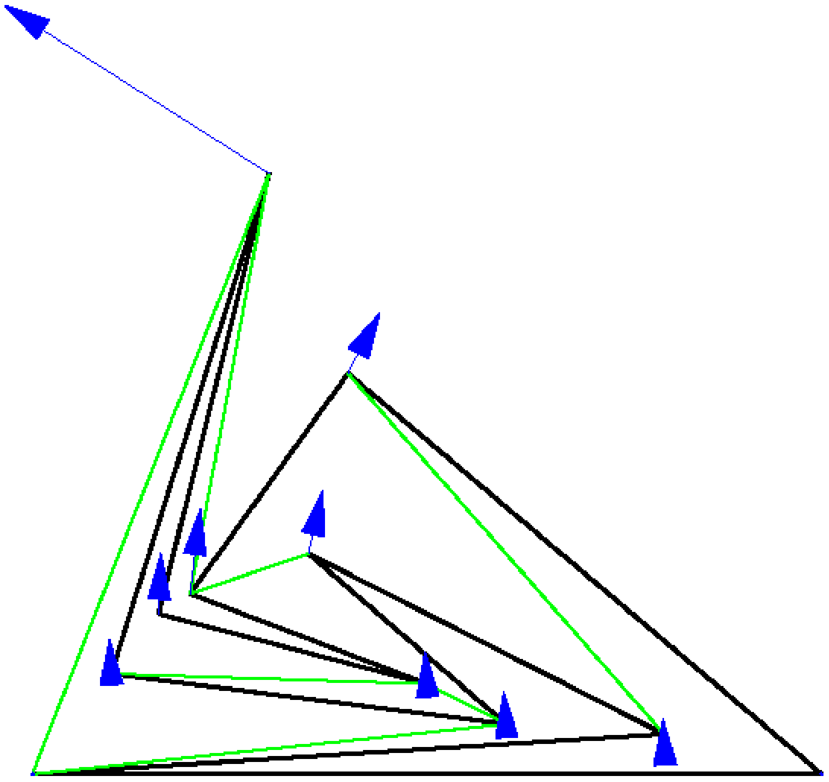
How to generate a meaningful Expansive Motion?



ODE-based:
From Erik Demaine's web page
http://db.uwaterloo.ca/~eddemain

Pseudo-triangulation based:
From my web page
http://cs.smith.edu/~streinu

Expansive *instantaneous* motions can be found using Linear Programming



- Assign velocity vector v_i to each vertex p_i
- Condition to keep some edges rigid: linear equalities

$$(p_i-p_j).(v_i-v_j)=0$$

- Condition to increase all other distances: linear inequalities

$$(p_i-p_j).(v_i-v_j) >= 0$$

- Add extra constraints to rule out trivial motions:

$$v_1^1 = v_1^2 = v_2^1 = 0$$

- Solve with Linear Programming

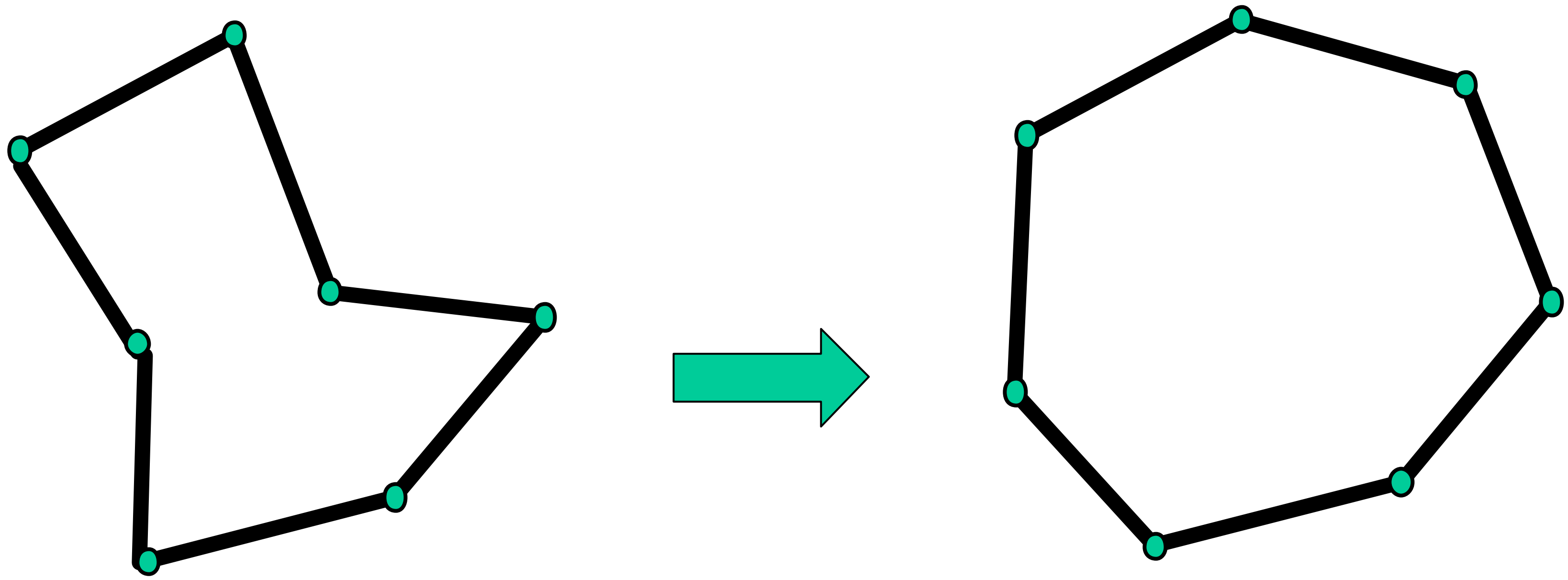
Pseudo Triangulations (missing a CH edge) correspond to special (canonical) basic feasible solutions

This gives the local “planner” of the motion. However:

Linear Programming is a very powerful, very general tool: one of the two top most used algorithms of the 20th century

- But is it REALLY necessary to rely on it?
- Can’t we solve it in a more intuitive (and efficient) way?

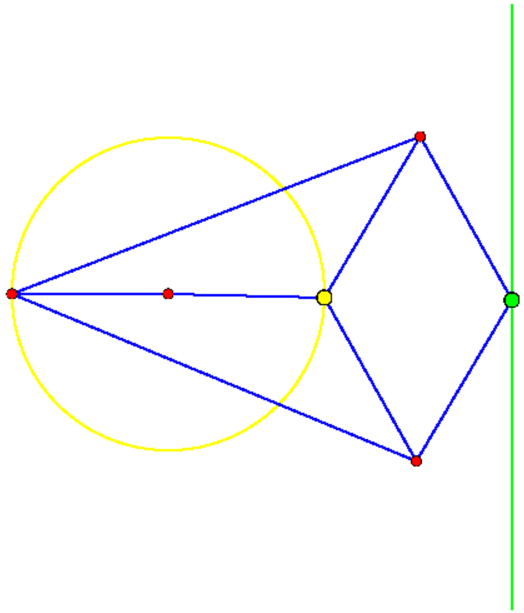
Main Result on PseudoTriangulations for the Carpenter's Rule Problem (IS'00)



A simple (open or closed) planar robot arm can be unfolded to a convex position (and hence reconfigured to any other similarly oriented position) with a sequence of at most $O(n^3)$ non self-intersecting, expansive motions induced by 1Degree-Of-Freedom mechanisms defined from pseudo triangulations.

Idea: decompose the trajectory into Simple Motions

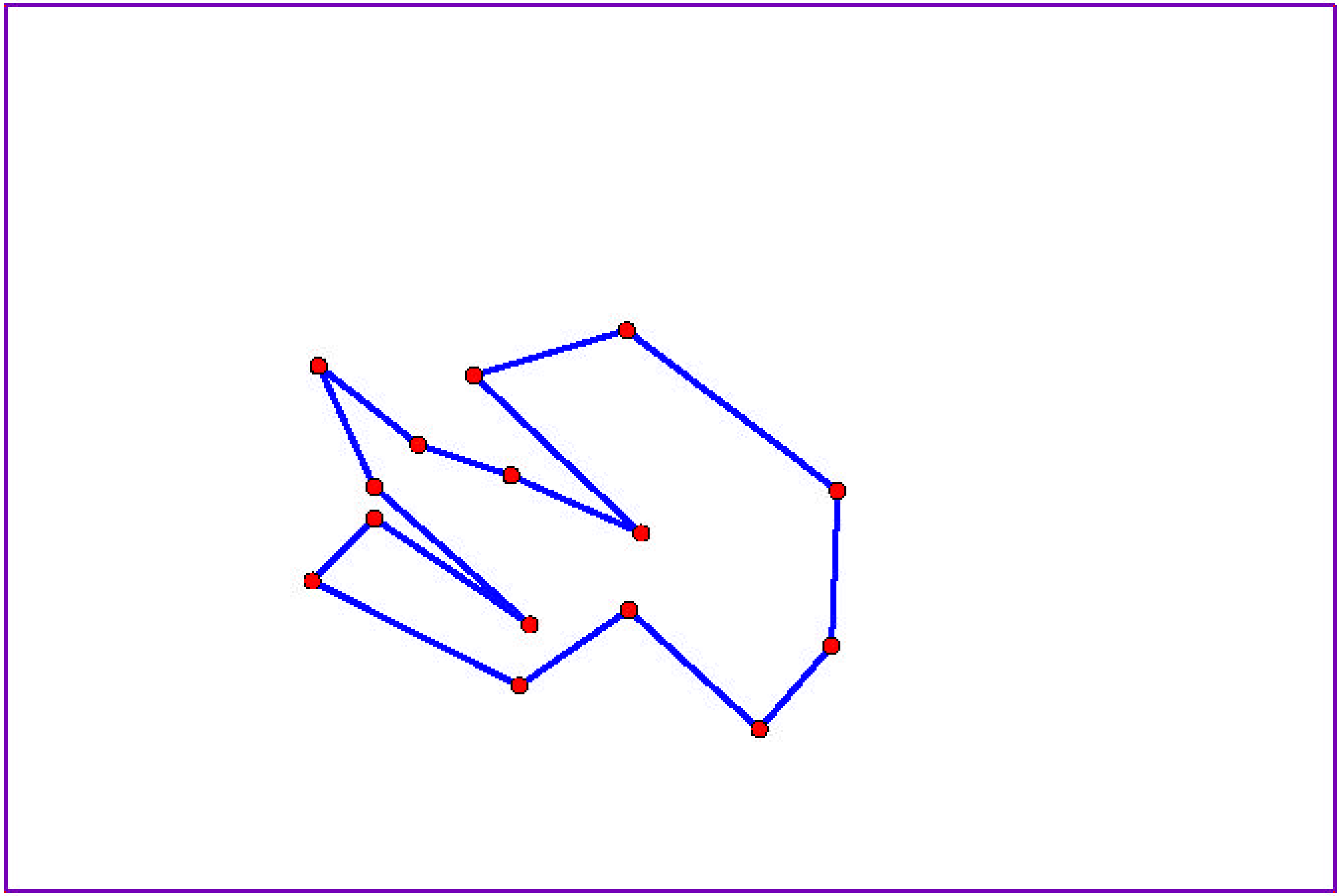
Use One Degree of Freedom Mechanisms



Example:

Peaucellier's linkage, 19^{th} century

Preview of the pseudo-triangulation technique:



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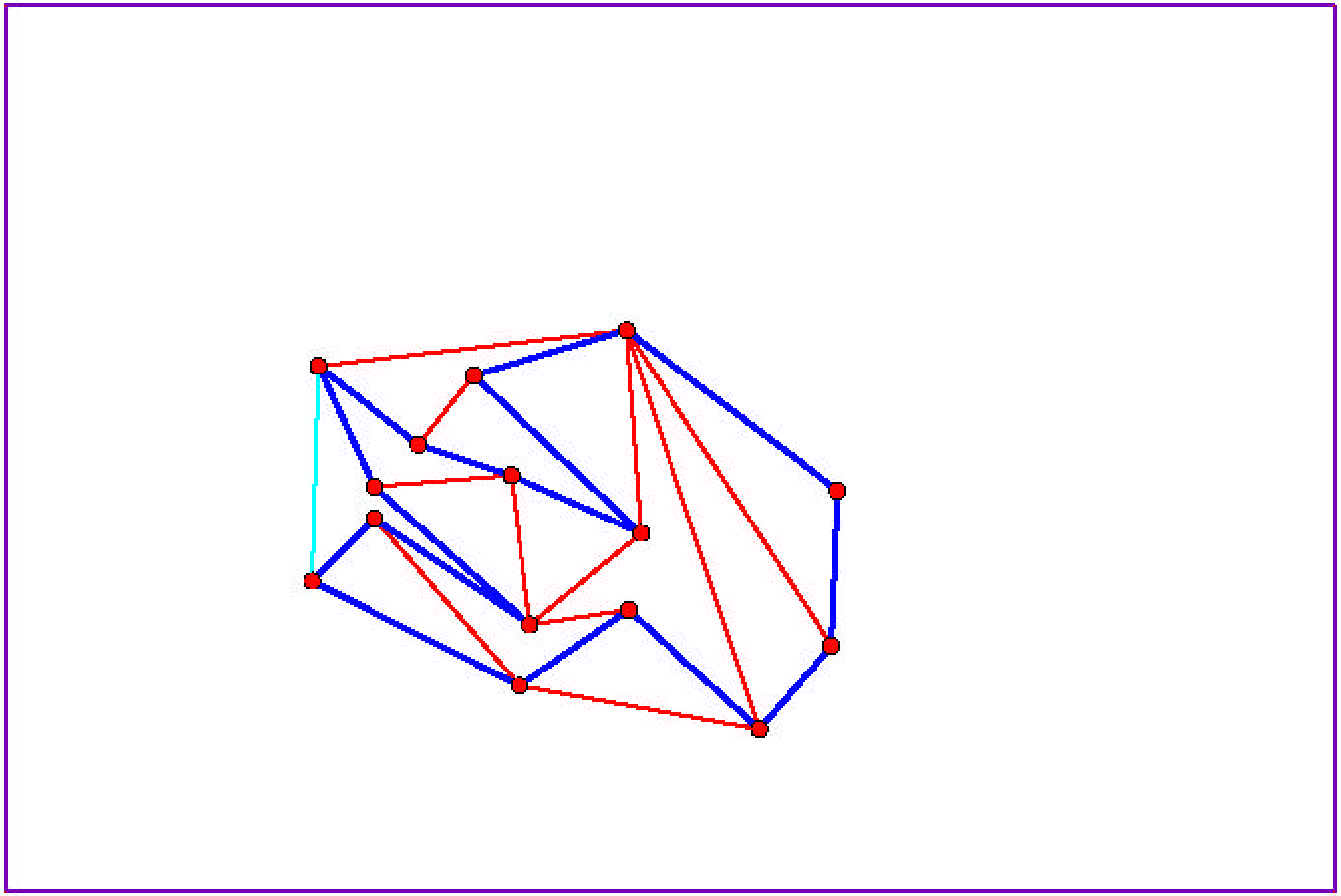
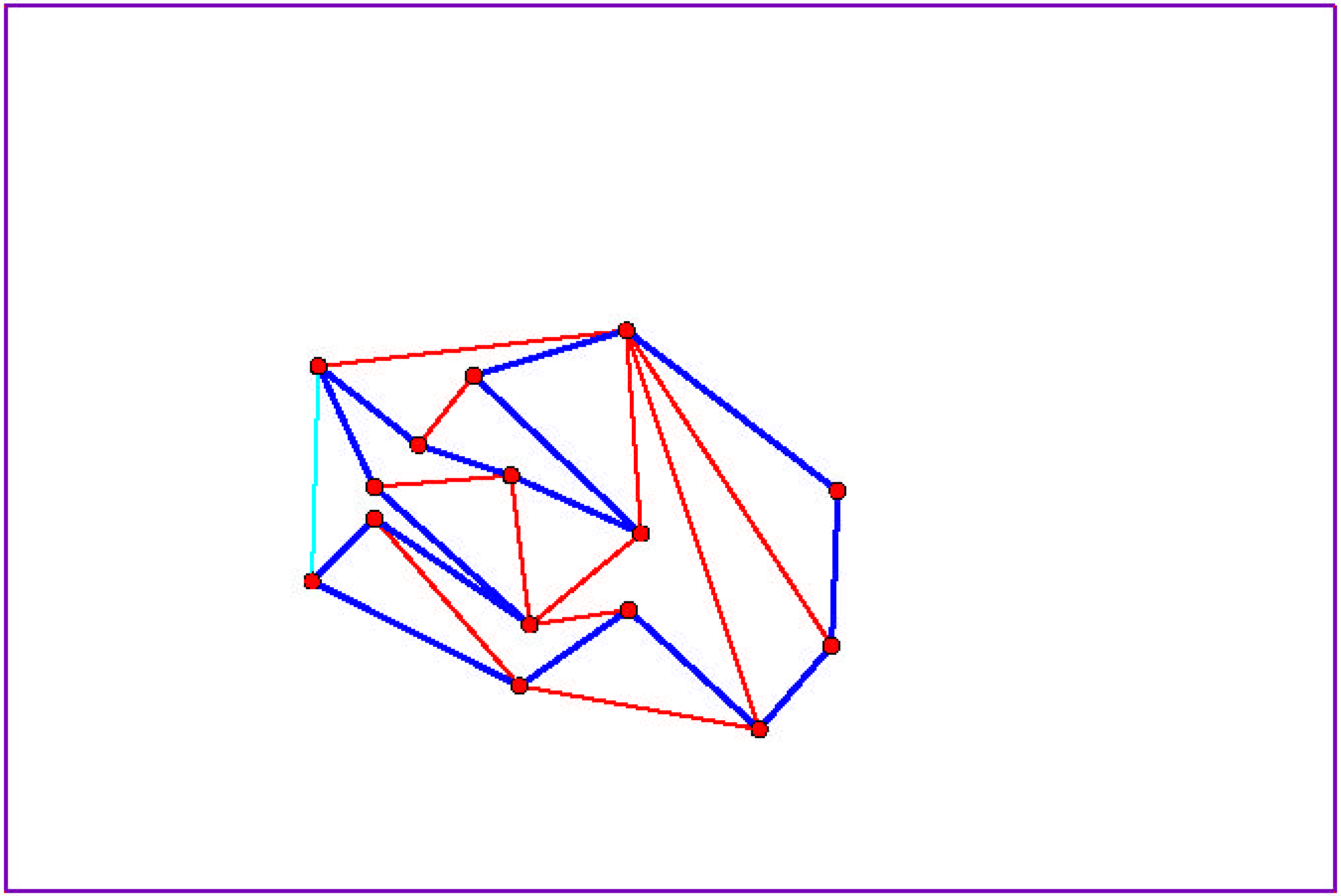
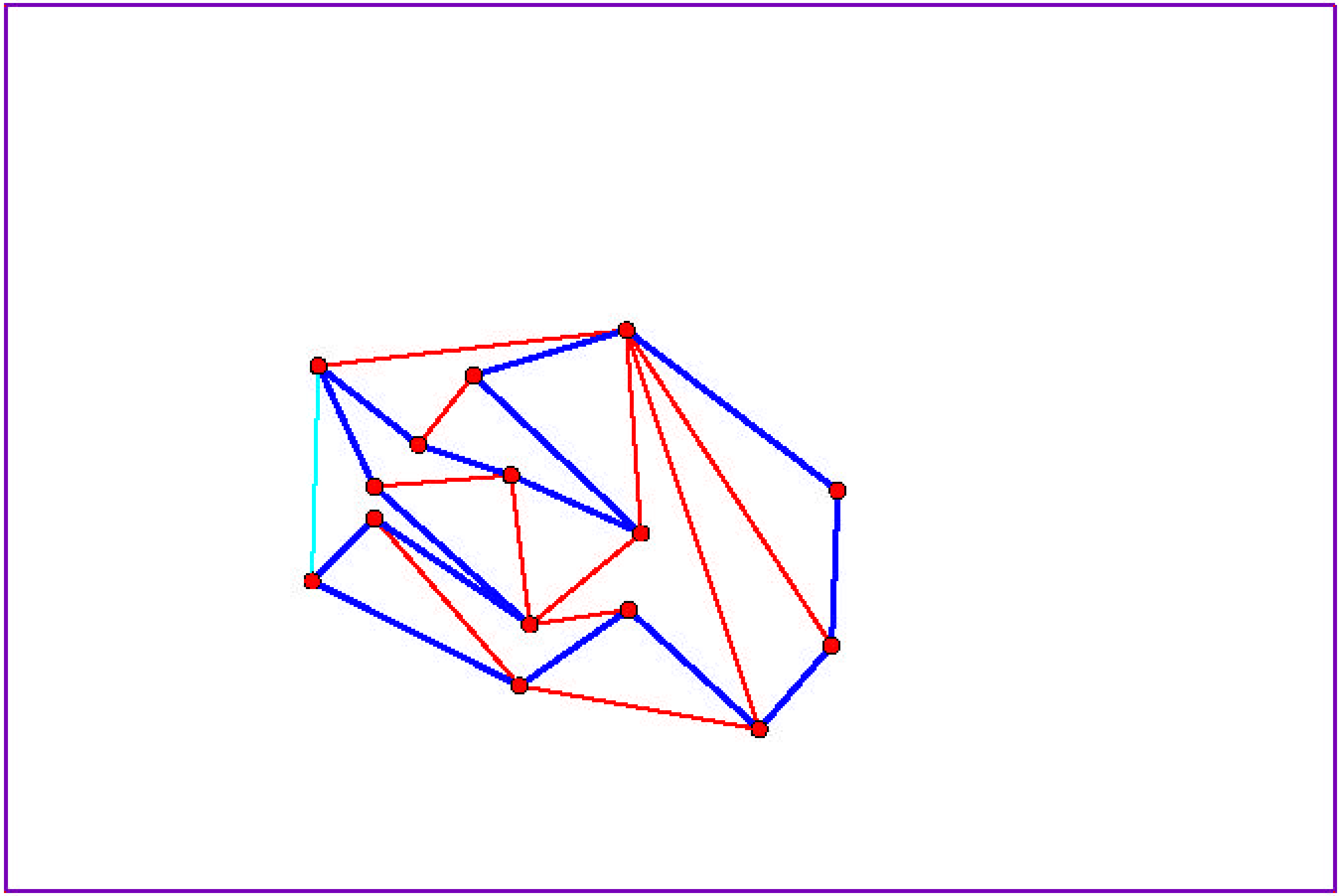
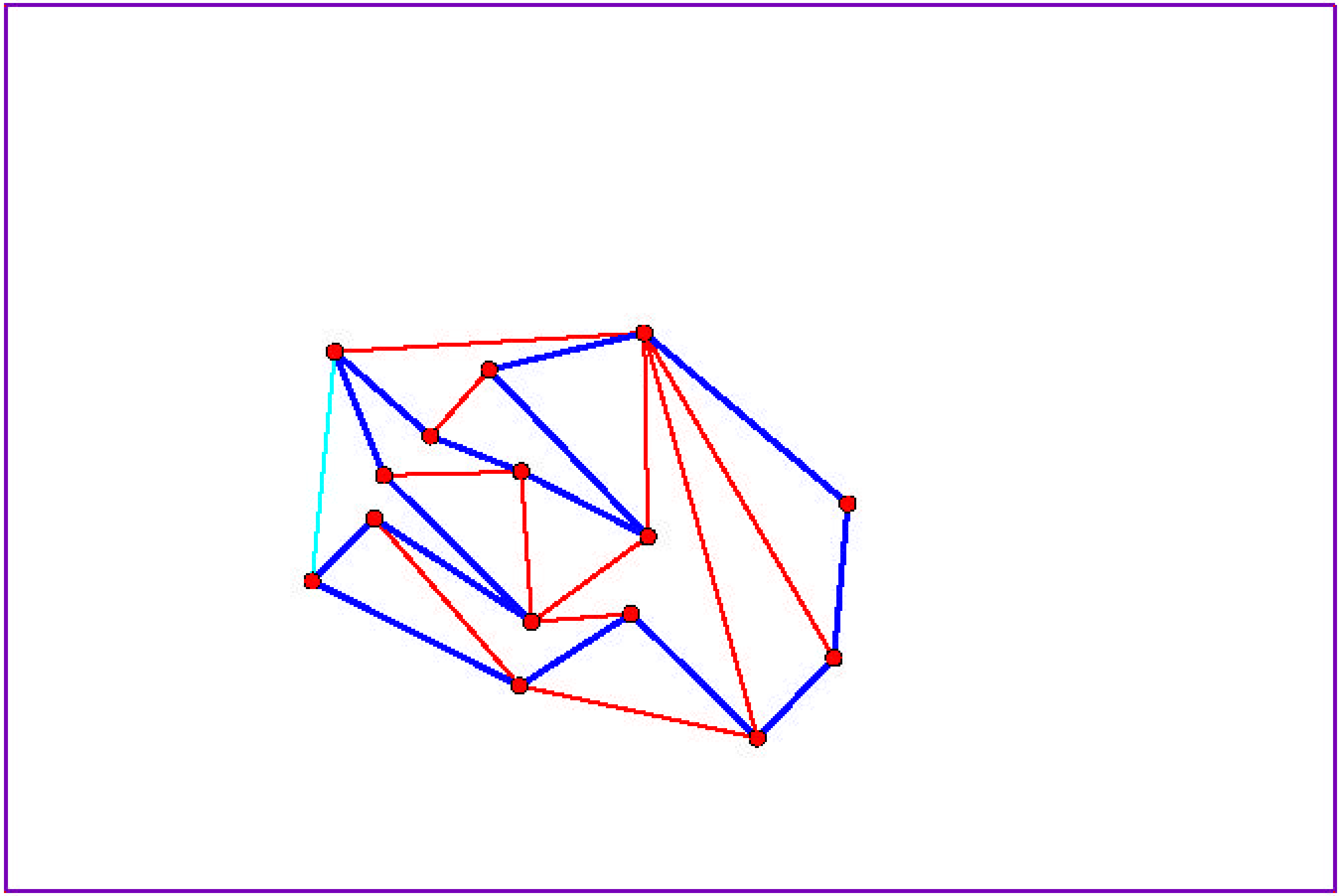


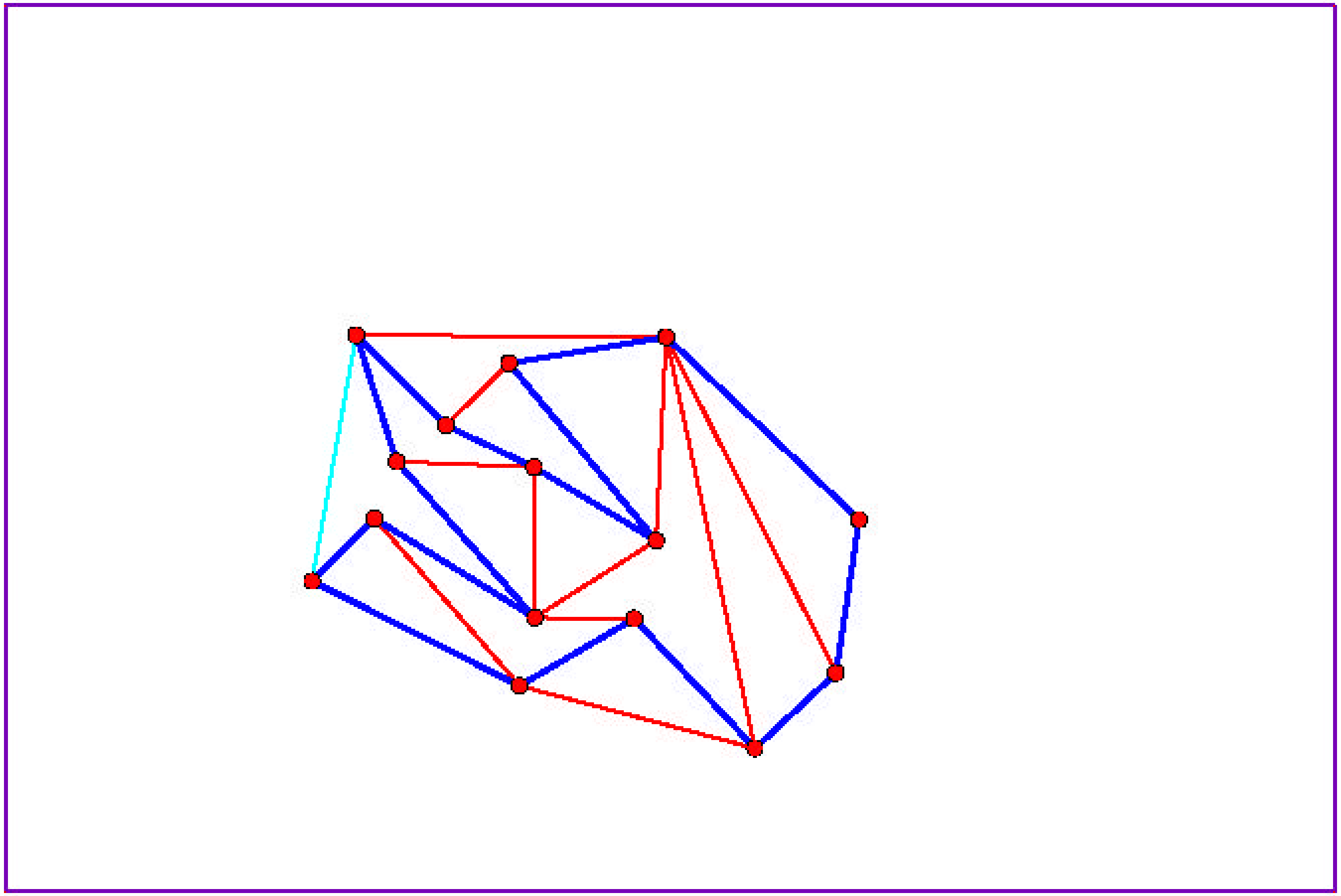
Add bars to restrict the motion: the more bars, the less freedom you have

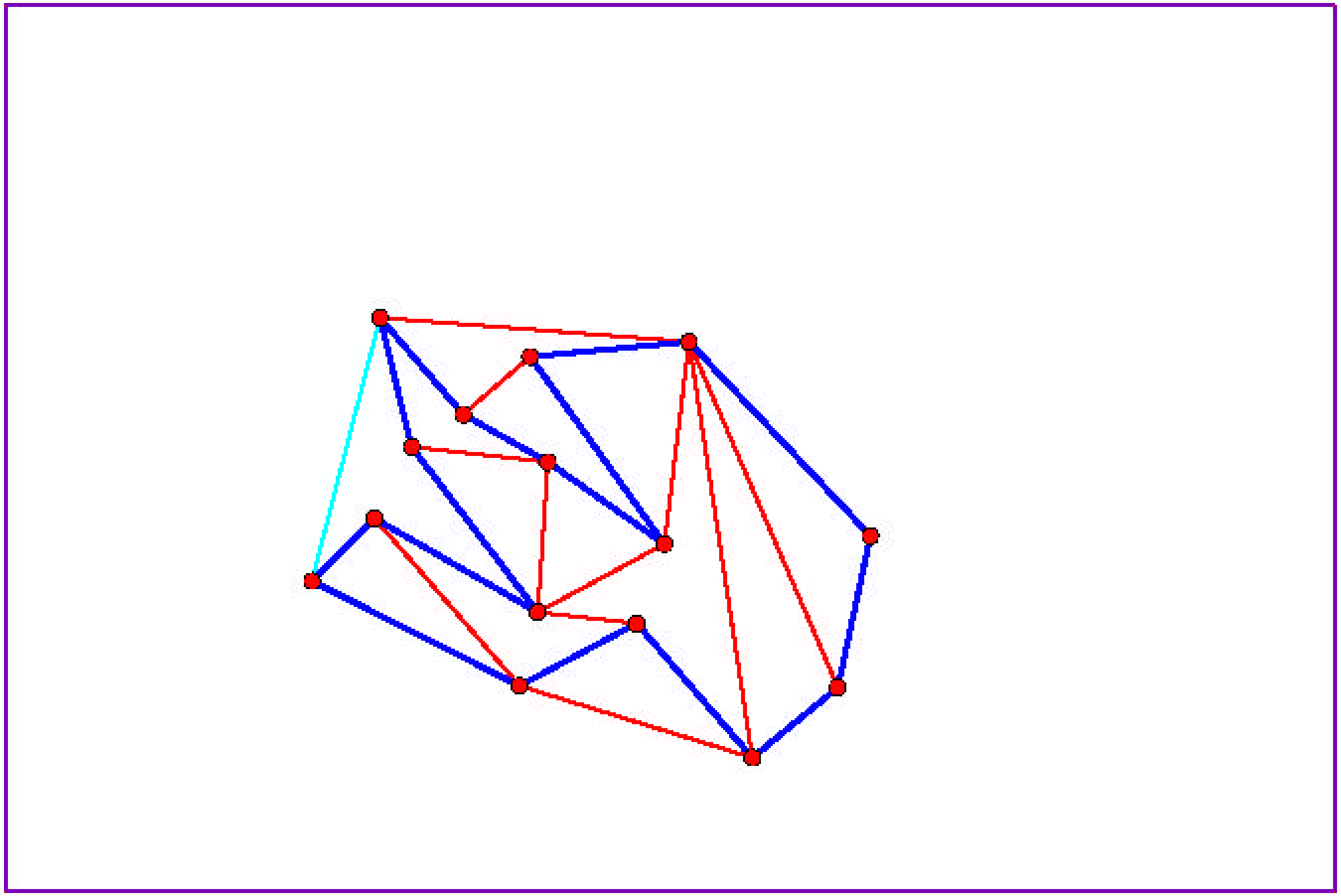
Bars placed in such a way that they "almost" form a pseudo-triangulation guarantee that the motion has only 1-degree-of-freedom and is expansive

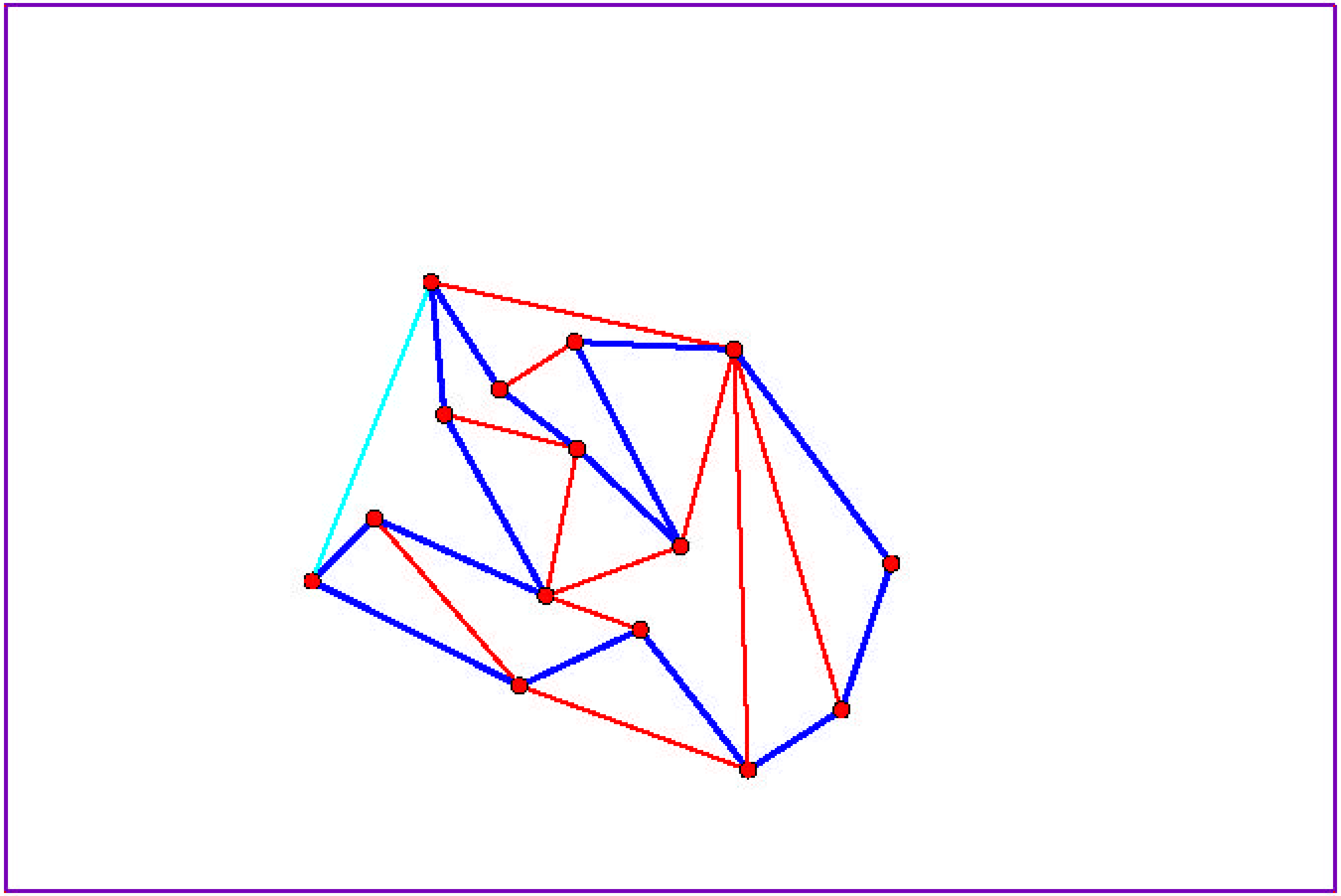


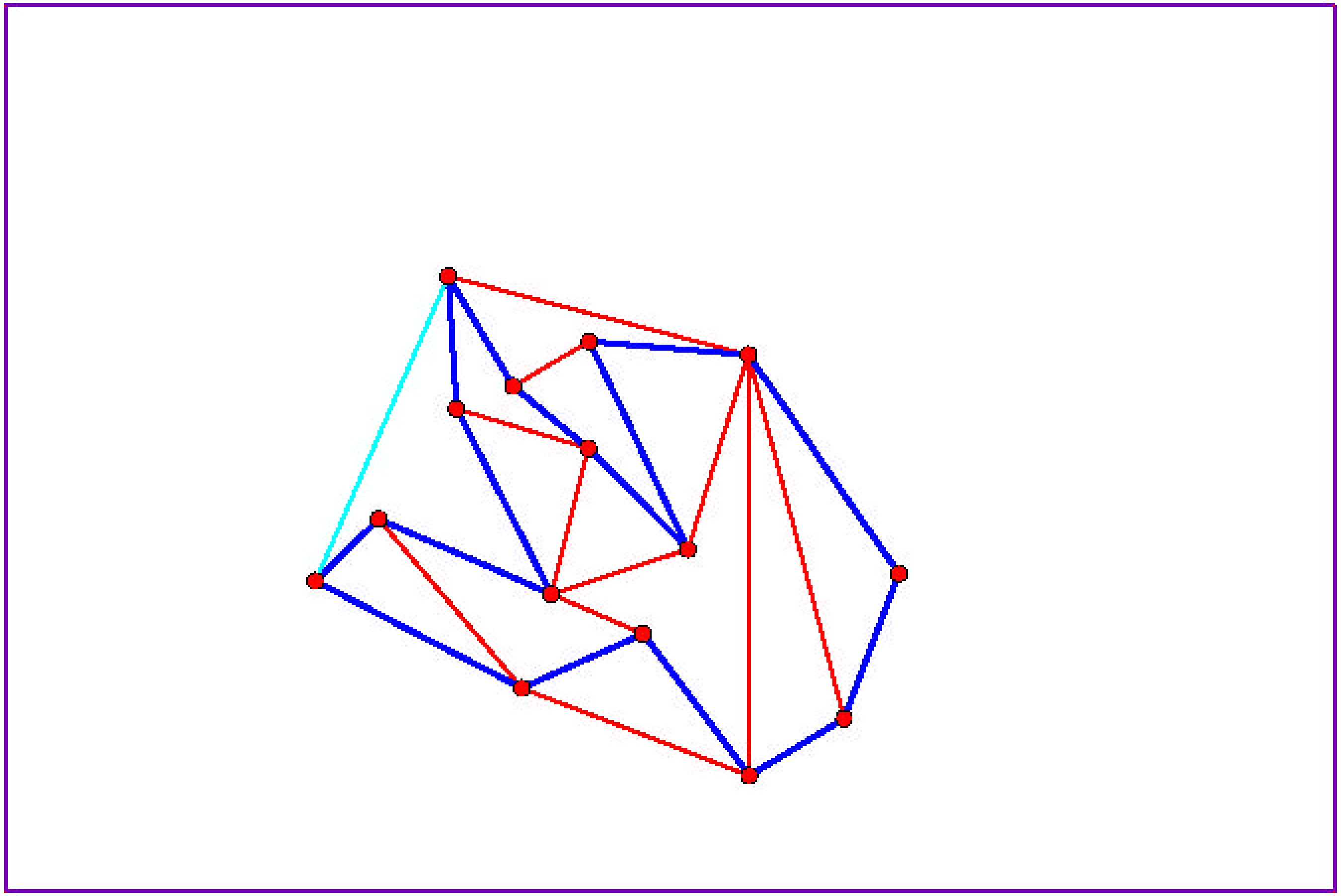




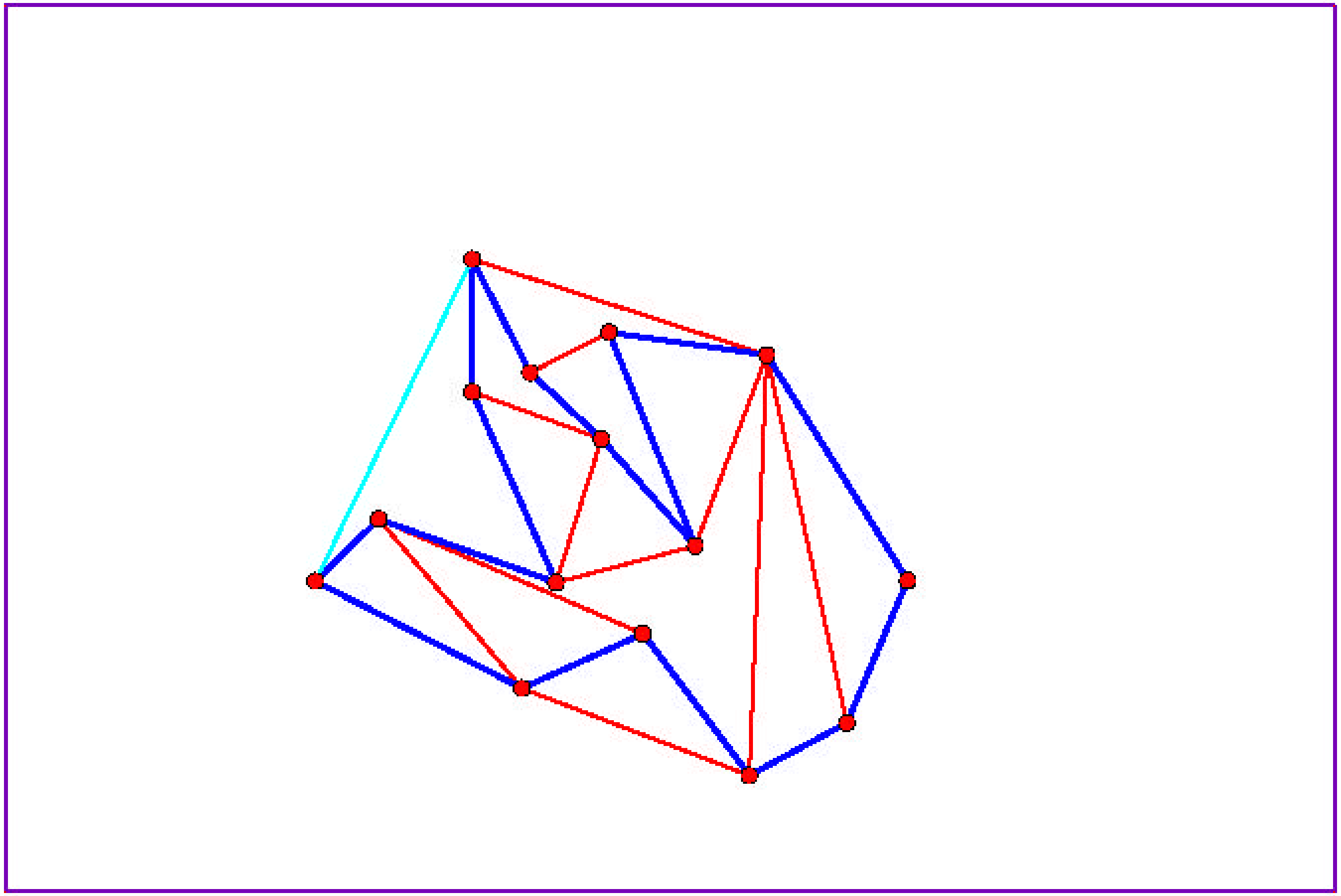




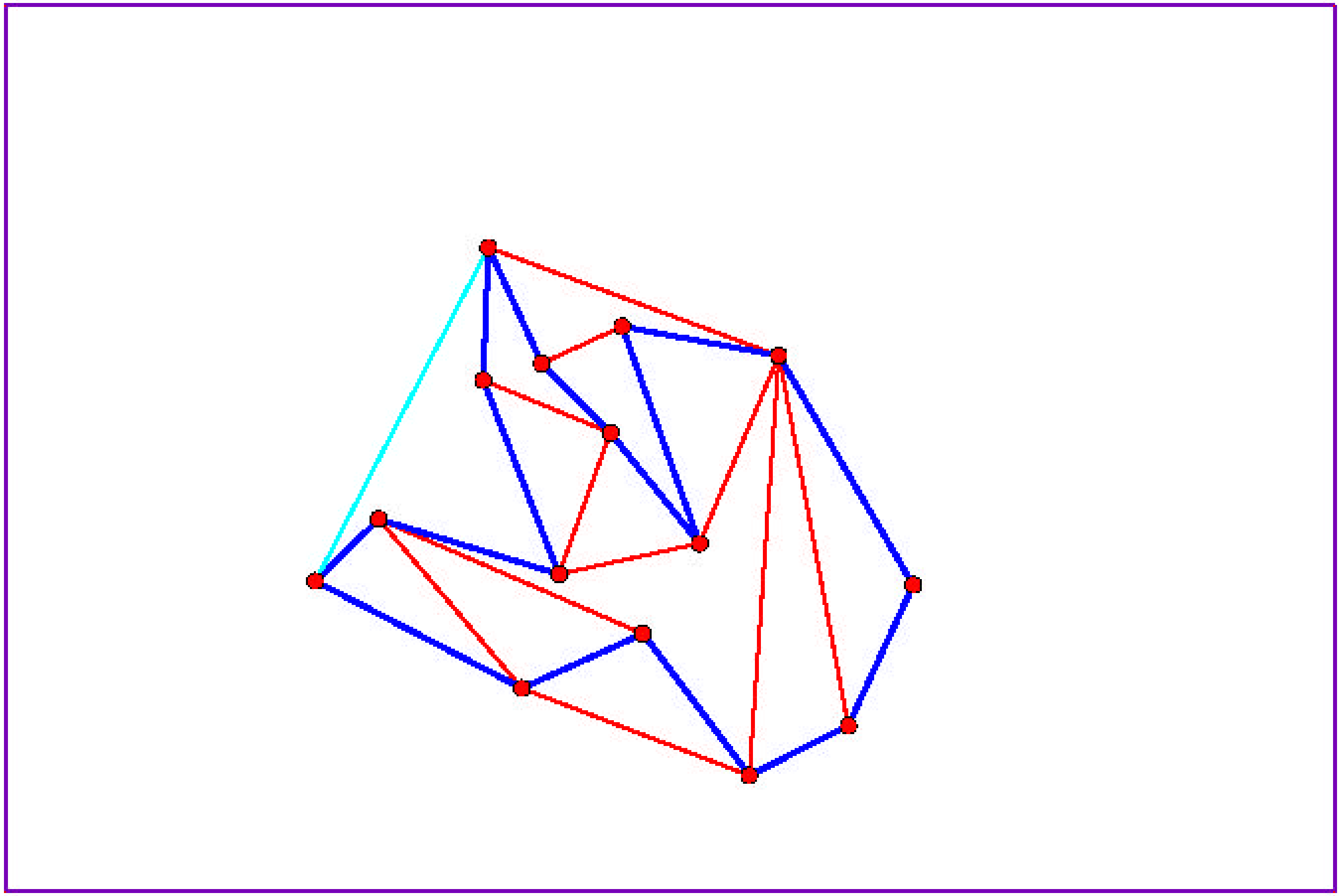


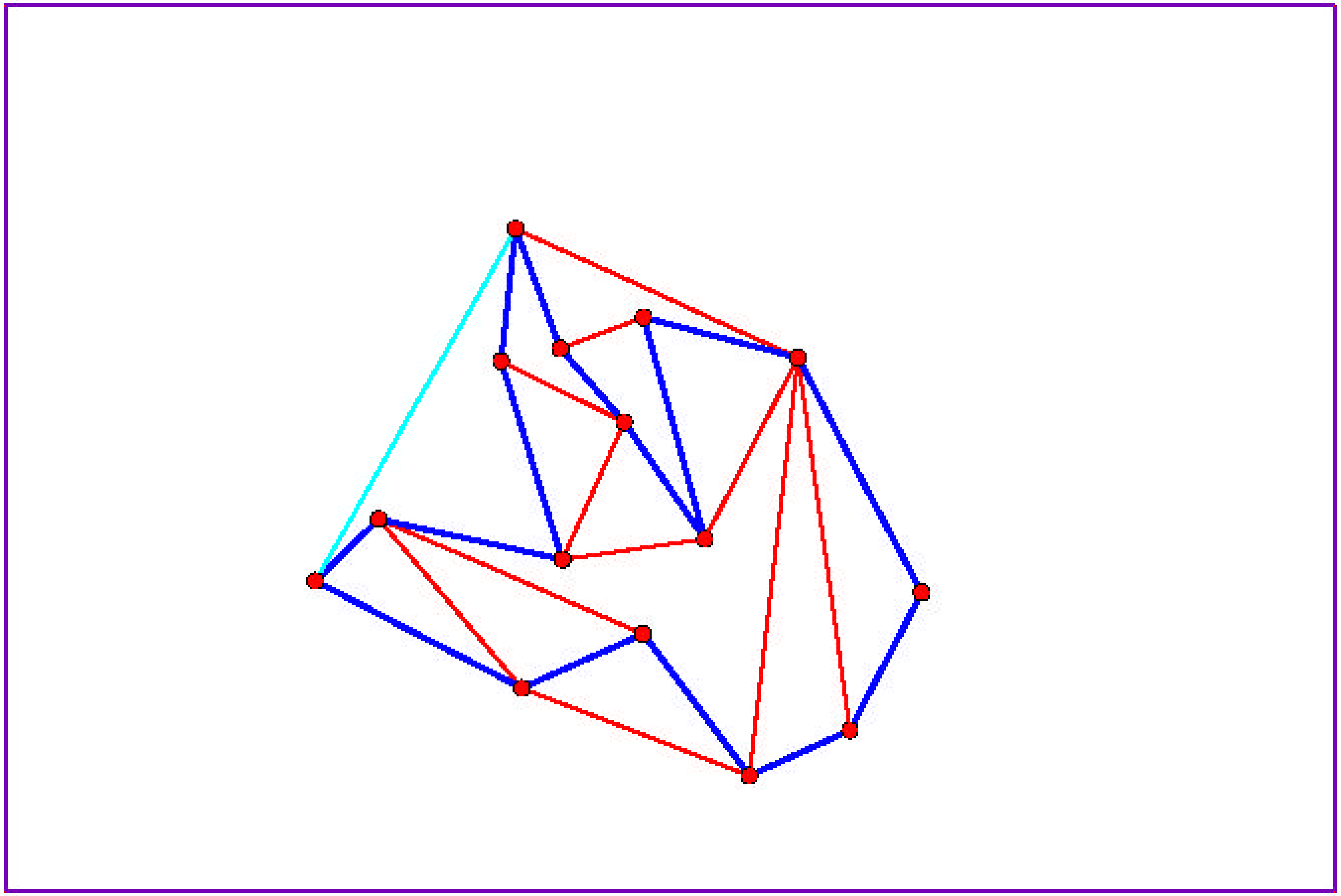


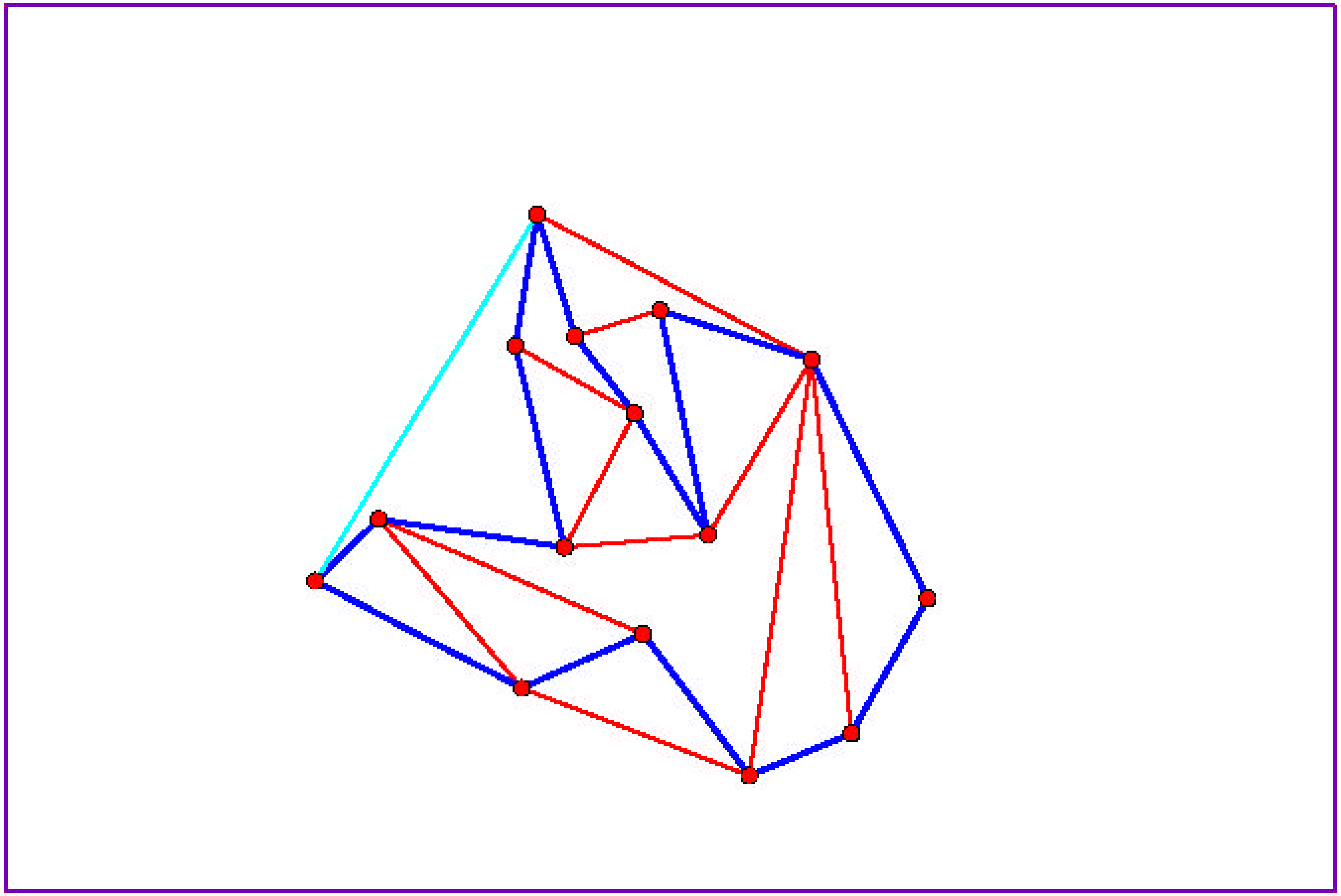
Events: alignment of adjacent bars

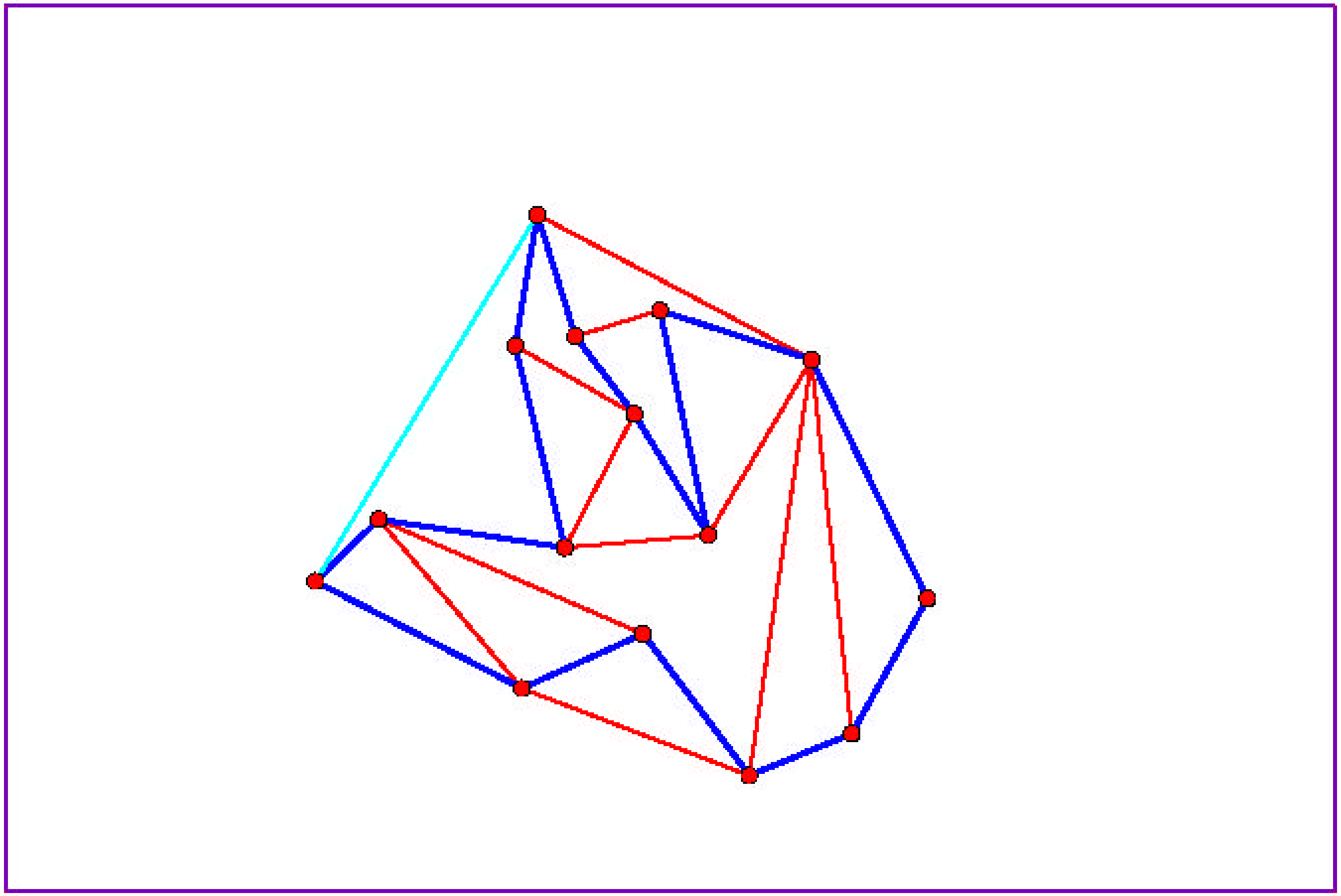


Readjust the mecahnism to maintain expansiveness









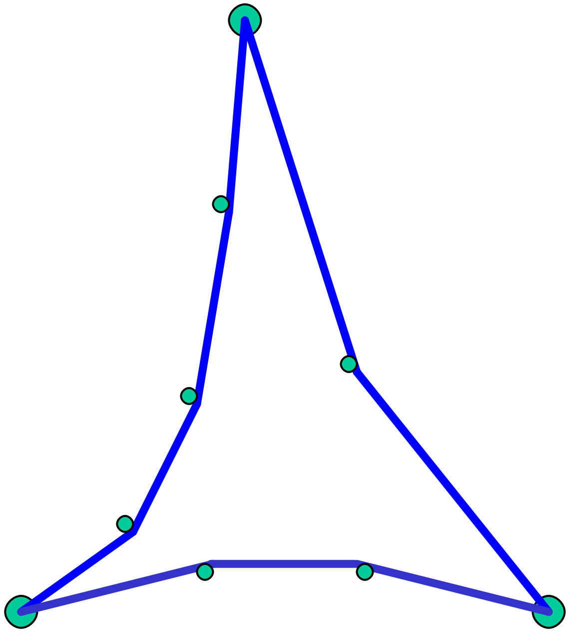
Show Cinderella mechanism

Definitions

- Pseudo-Triangle
- Pointed Collection of Bars
- Pseudo-Triangulation

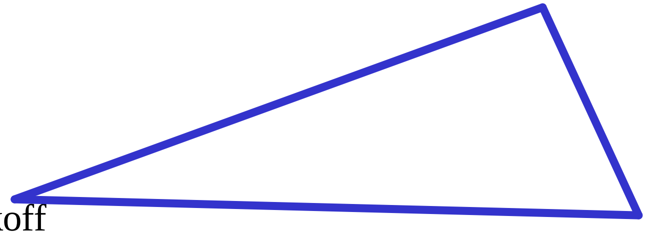
Rigid structure with oriented matroid information

Pseudo Triangle



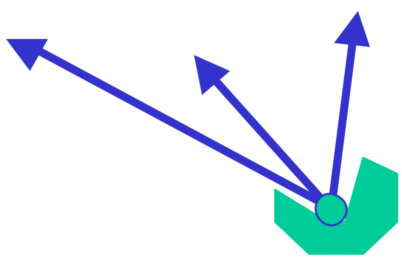
A simple polygon which has exactly three convex vertices.

In particular, a triangle is a pseudo-triangle.



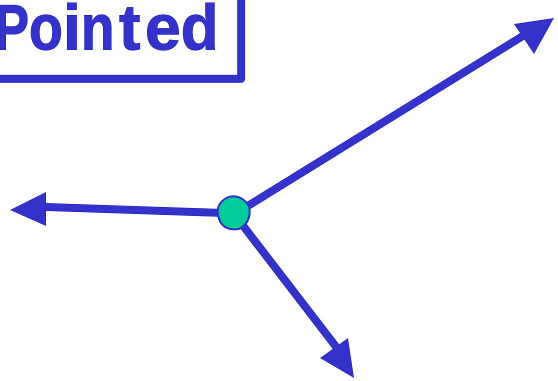
Pointed Planar Set of Vectors

Pointed

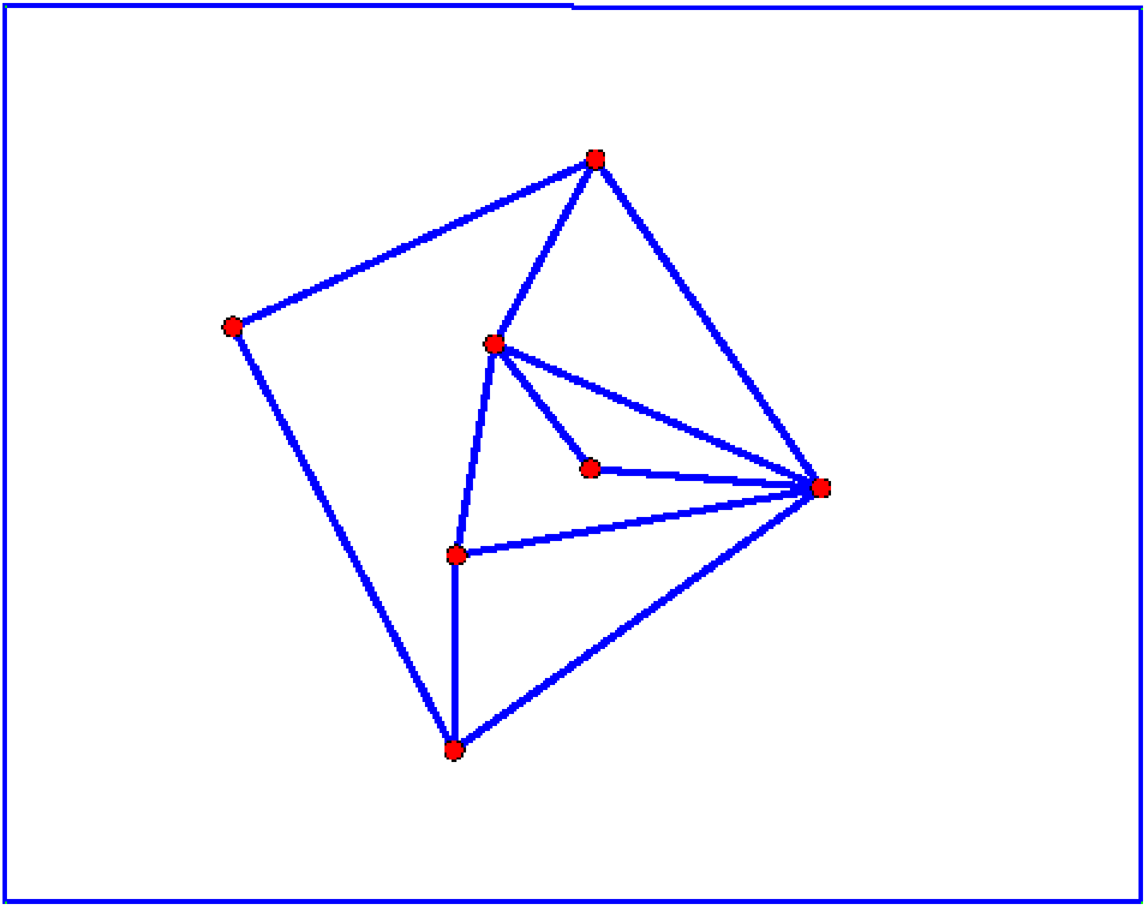


Span a **reflex angle**

Not Pointed



Pointed Pseudo Triangulation of a Planar Set of Points [IS'00]



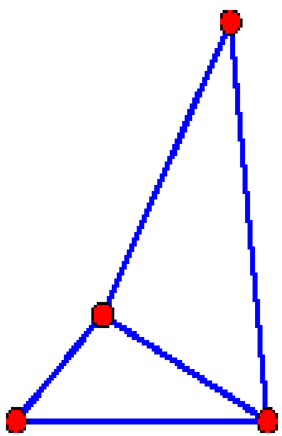
- Partitioning of the **convex hull** with a maximal set of **non-crossing** and **pointed** interior edges.
- The resulting faces are **pseudo-triangles.**

Pointed Pseudo Triangulations

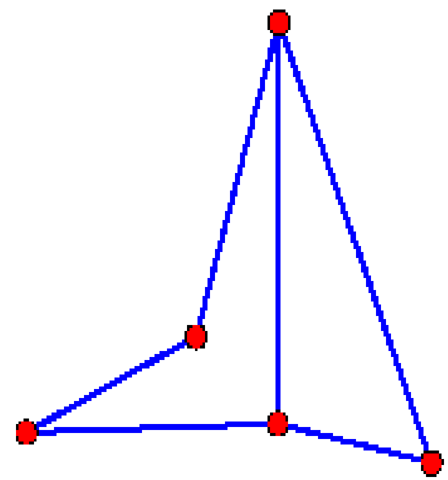
Are **minimally rigid**

- Infinitesimally, generically rigid
- Lots of useful combinatorial and rigidity theoretic properties: 2n-3 count, inductive construction, have a polyhedral representation

Rigid and Non-Rigid Graphs



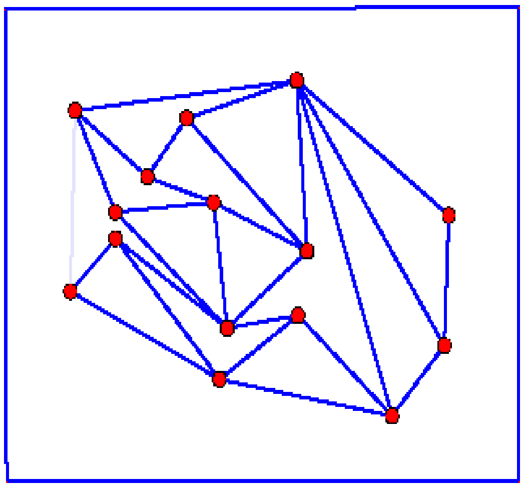
0 DOFS



1 DOF

Minimally rigid: removing any edge makes them **flexible**

Pseudo-triangulation mechanisms



A (pointed) pseudo triangulation without a convex hull edge is a 1DOF expansive mechanism (S'00).

Proof based on a theorem of Maxwell 1870's.

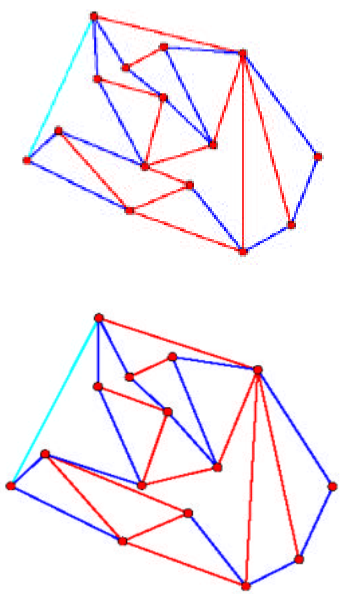
(show Cinderella mechanism 0)

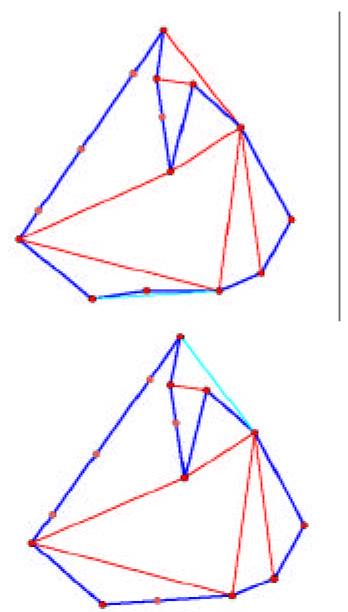
To complete the planning of the motion, we need Algorithms for:

- Constructing a Pseudo Triangulation
- Readjusting it by local flips at event points: when two adjacent edges align

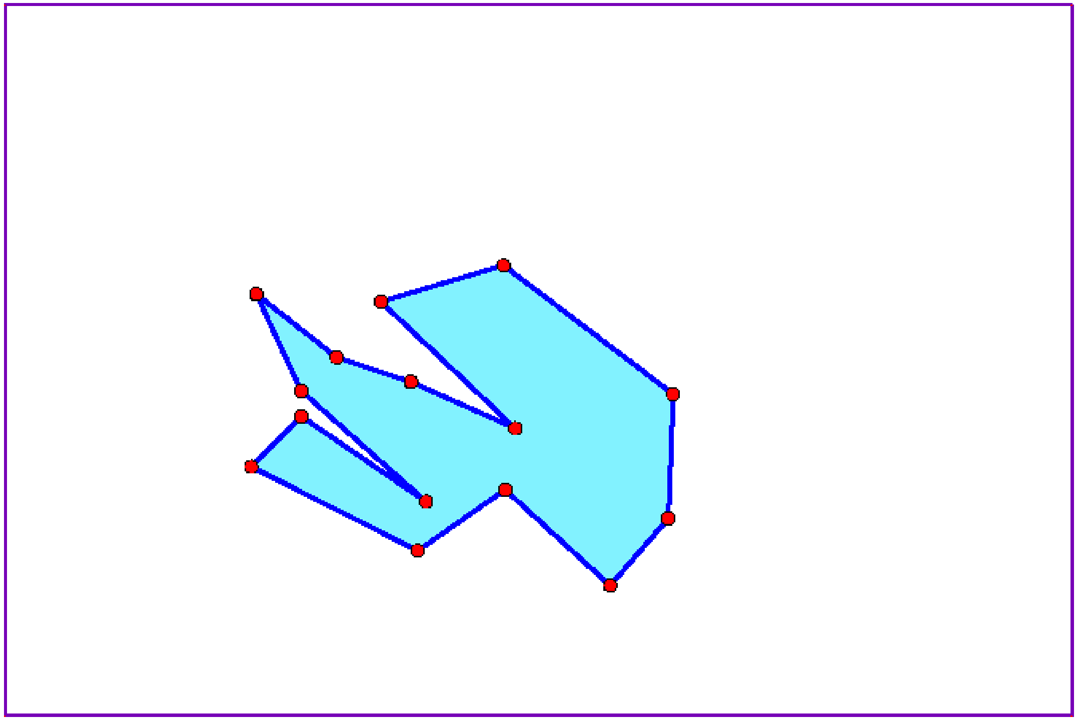
Readjusting Pseudo-Triangulations by Local Flips

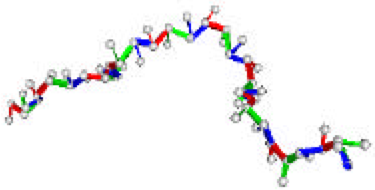
- Events: alignment of two adjacent edges
- Locally flip or freeze a vertex



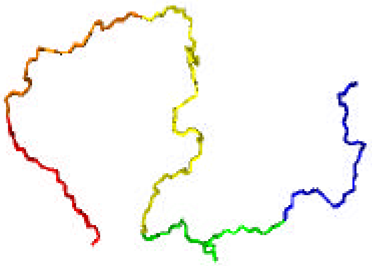


Putting everything together





Outline

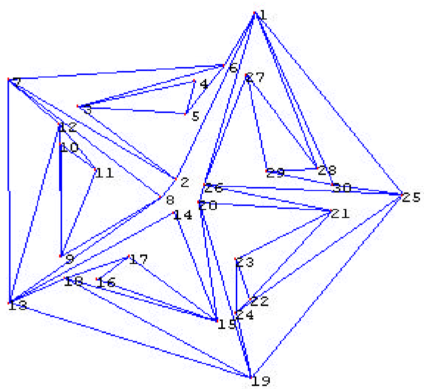


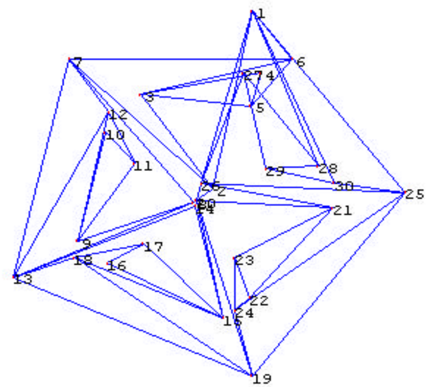
- Quick overview of existing approaches
- Quick overview of previous work of PI's related to the main theme of the project
- What we plan to do
- Overview of the pseudo-triangulation approach to the 2 dimensional problem
- Lessons learned from 2d
- Challenges in dimension 3

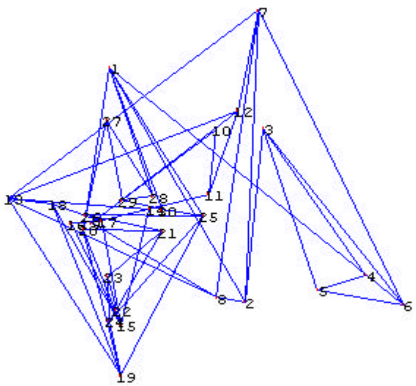
In reverse: folding processes

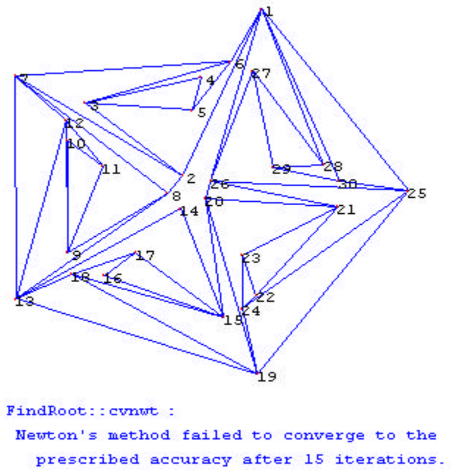
- Each pseudo-triangulation induces contractive motions ("attractive" forces)
- Readjustments at event points: when an angle at a corner of a pseudo-triangle becomes 0
- Partially folded states may be generated at random, or by physical considerations

Numerical Challenges: alignment events







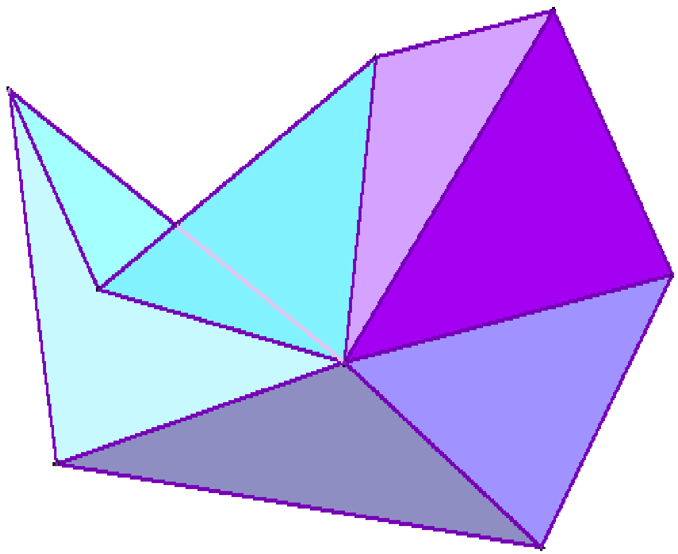


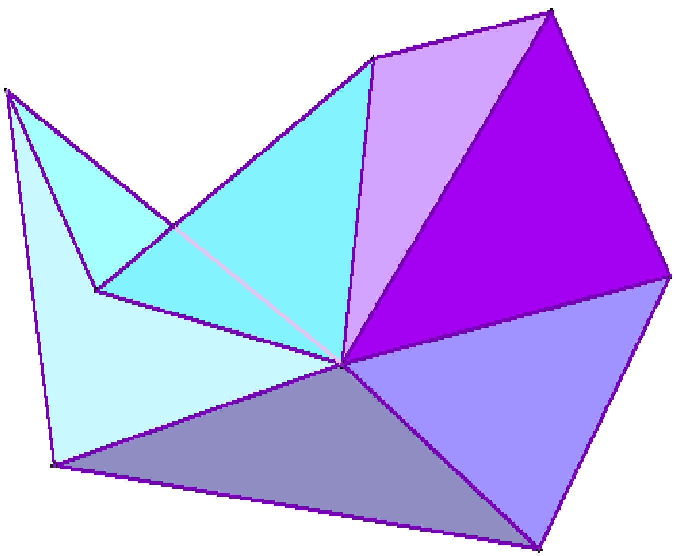
- Exact computation of alignment event: Groebner bases
- Iterative methods: slow convergence sometimes. Can that be predicted combinatorially?
- Useless computations that can be pruned with rigidity theory tools: rigid components (Cinderella mechanism m2)

Another Application

Conical Folding of a Flat Piece of Paper

has the same geometry as the planar Carpenter's Rule Problem





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- Self-crossings disallowed.

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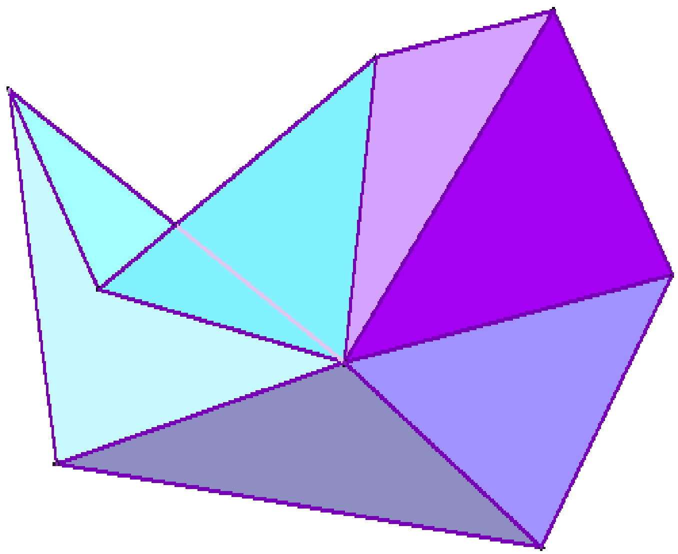

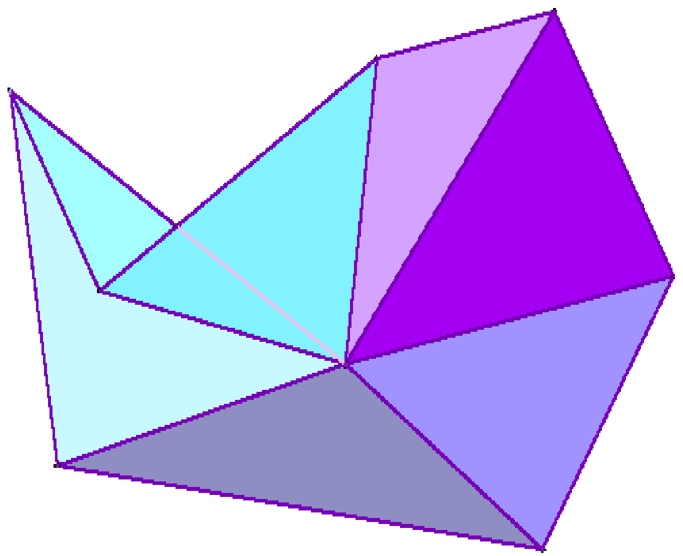

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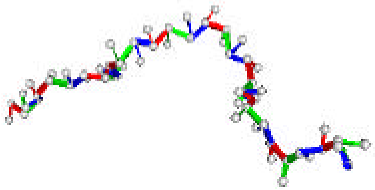
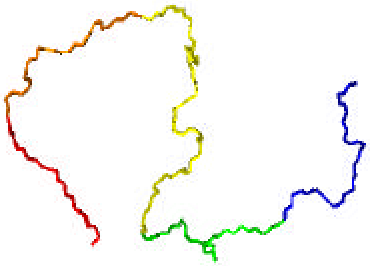


Outline



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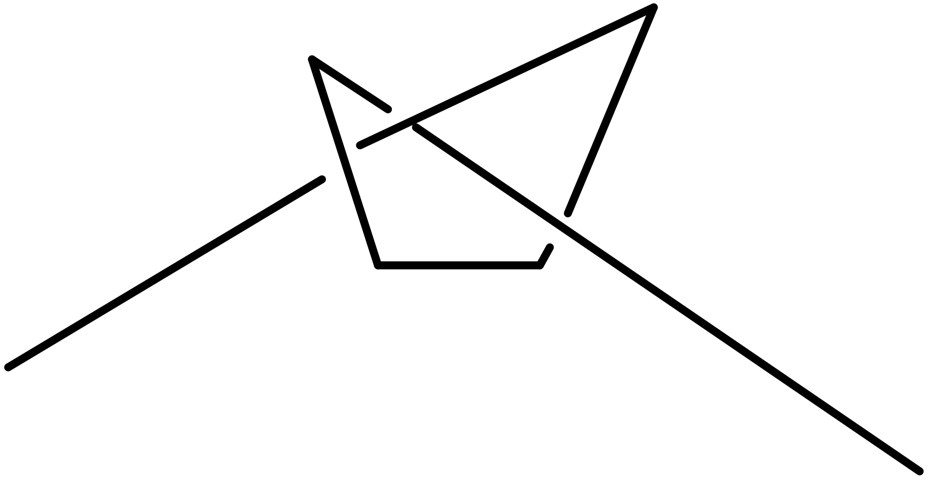
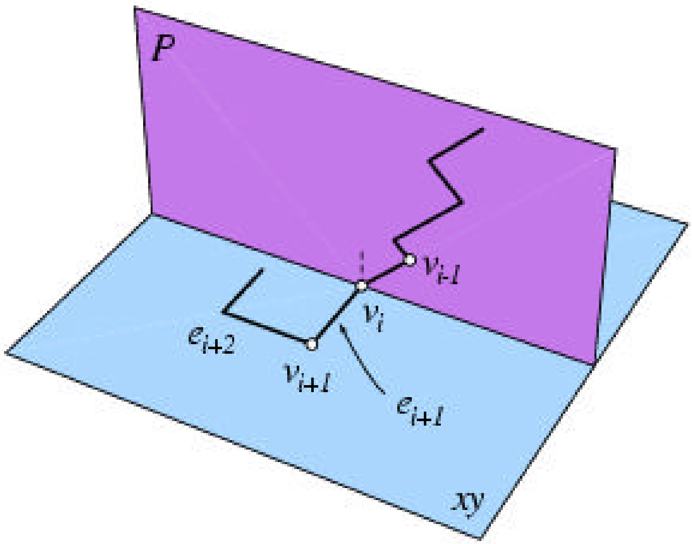
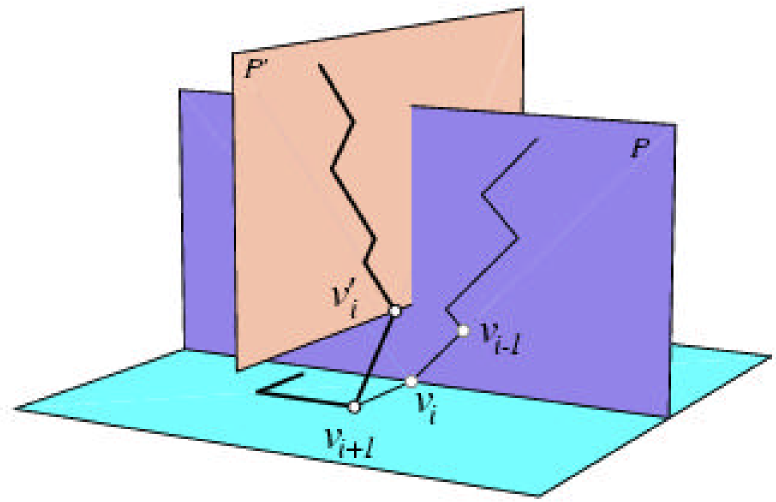
Challenges for Spatial Linkages



- R^3: reconfiguration not always possible
- Unknotted polygon that cannot be convexified without self -intersections, BDD+ 1998, CJ'98.

Recent Work on 3d Flat Linkages with Fixed Angles





- Aloupis, Demaine, Langerman, Meijer, O'Rourke, Overmars, Soss, Streinu, Toussaint '02: polynomial results on open chains with equal sides or special equal acute angles, orthogonal, open and closed chains.

Our Proposed Mathematical and Algorithmic Approach

(beyond the range of this one year CARGO Incubation Grant)

Study the topology and algorithmics of

folding processes of 2d and 3d linkages

Goal: Develop a discrete (combinatorially described) partitioning of configuration space which may be more easily sampled to generate candidates for folded states

- Use recently developed ideas from 2d based on Pseudo-triangulations and Rigidity Theoretical tools
- Tools: "3d pseudo-triangulations"?
- Simplify the numerical computations using tools from combinatorial Rigidity Theory
- Explore potential parallelism

Questions?